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THESIS

NUMERICAL SOLUTION OF SECOND ORDER

DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ APPROXIMANTS

* * * * *

William B. [illegible], Jr.

NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ CONVERGENTS

* * * * *

William B. Moye, Jr.

NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ COEFFICIENTS

by

William B. Moyo, Jr.

Lieutenant Commander, United States Navy

Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE

United States Naval Postgraduate School
Monterey, California

1966

NUMERICAL SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS USING RATIONAL PADÉ CONVERGENTS

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This work is accepted as fulfilling
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from the

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ABSTRACT

Rational Padé convergents to a function of the forward shift operator E are computed from coefficients of its power series expansion. These Padé convergents are used to generate recursion formulas which are then employed to obtain approximate numerical solutions of several second order differential equations. A variety of integration step lengths are used. Solution error is plotted against the number of iteration steps and results are evaluated. It is concluded that this procedure is beneficial as a method of deriving corrector formulas to be used in the predictor-corrector method of solving second order differential equations. A method for deriving improved predictor formulas is suggested.

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1. Introduction.

Kopal [3] has suggested a numerical method for solving differential equations which uses rational Pade convergents to approximate functions of the forward shift operator E to generate recursion formulas. He has demonstrated the merits of using such formulas in solving first order equations and has exhibited certain stability problems related thereto.

The purpose of this paper is to extend the study of this method in the special category of second order differential equations in which the first derivative does not appear. A computer program is developed which generates a number of recursion formulas, applies them successively to solve the initial value problem $y'' + y = 0$, $y(0) = 1$, $y'(0) = 0$, and produces graphs of solution error vs number of iterations. The basic program is then modified to solve the Coulomb Wave Equation $y'' + y\left(1 - \frac{2\eta}{x} - \frac{L(L+1)}{x^2}\right) = 0$ with initial conditions appropriate to the selected values of the parameters η and L. The Runge-Kutta method is used to compute eight values of the independent variable to start the solution. Finally, the results of these computations are discussed in detail.

Some of the advantages of this method over others in common use are:

a. A rational convergent is generally a better approximation to a function than is the corresponding truncated series. This will be discussed further in the following section.

b. Only about one half the total number of tabular differences required by methods using polynomial approximations are needed in this method for comparable accuracy. This is because differences are distributed over both sides of the recursion formula.

c. Since differencing is divided between both sides of the

equation, neither side is differenced too many times. This reduces the number of computations required and, consequently, the round off error.

4. Recursion formulas derived from Padé convergents are extremely easy to generate in a digital computer program. This will be illustrated in Section 6.

2. Derivation of Recursion Formulas.

Suppose it is desired to solve the initial value problem

$$y''(x) = f(x,y(x)), \quad y(x_0) = y_0, \quad y'(x_0) = y_0'. \qquad (1)$$

Integrating formally on each side

$$\int_{x_0}^{x_0+mh}\int_{x_0}^{t} y''(\xi)\,d\xi\,dt = \int_{x_0}^{x_0+mh}\int_{x_0}^{t} f(\xi, y(\xi))\,d\xi\,dt$$

we get on the left side

$$\int_{x_0}^{x_0+mh} (y'(t) - y'(x_0))\,dt = y(x_0+hm) - y(x_0) - y'(x_0)hm .$$

Introducing a change of variable

$\xi = x_0 + hz_1, \qquad d\xi = h\,dz_1$

$t = x_0 + hz, \qquad dt = h\,dz,$

and defining the forward shift operator E such that $E^m f(x) = f(x+mh)$, we get on the right (treating E as an algebraic symbol):

$$h^2\int_0^m\int_0^z f(x_0+hz_1, y(x_0+hz_1))\,dz_1\,dz = h^2\int_0^m\int_0^z E^{z_1} f(x_0,y_0)\,dz_1\,dz$$

$$= h^2\int_0^m \left[\frac{E^{z_1}}{\ln E}\right]_0^z dz = \frac{h^2}{\ln E}\int_0^m (E^z - 1) f_0\,dz = \frac{h^2}{\ln E}\left\{\left[\frac{E^z}{\ln E} - z\right]_0^m\right\} f_0$$

$$= \frac{h^2}{\ln E}\left\{\frac{E^m}{\ln E} - \frac{1}{\ln E} - m\right\} f_0 .$$

Finally, $$y_m - y_0 - hm\,y_0' = \left(\frac{h}{\ln E}\right)^2 \left\{E^m - 1 - m\ln E\right\} f_0 .$$

or, [illegible]

Assuming we know f_i $i=1,\dots,m$ we can write

$$y_{m+i} = \left(\frac{h}{\log E}\right)^2 f_{m+i} + y_0 + h(m+i)\,y_0' - \left(\frac{h}{\log E}\right)^2 \left\{ f_0 + \left[(m+i)\log E\right] f_0 \right\}.$$

Setting i = 1 $\qquad y_{m+1} - y_m = \left(\frac{h}{\log E}\right)^2 \left\{ f_{m+1} - f_m \right\} + h y_0' - \frac{h^2}{\log E} f_0$, or

$$(E-1)\,y_m = \left(\frac{h}{\log E}\right)^2 (E-1) f_m + h y_0' - \frac{h^2}{\log E} f_0\,, \quad y_m = \left(\frac{h}{\log E}\right)^2 f_m + \frac{h}{E-1} y_0' - \frac{h^2}{\log E}\frac{f_0}{E-1}.$$

In terms of the backward difference operator ∇, defined by $\nabla y_i = y_i - y_{i-1}$, this is

$$y_m = \left\{\frac{h}{-\log(1-\nabla)}\right\}^2 f_m + h\,\frac{(1-\nabla)}{\nabla}\,y_0' - \frac{h^2}{-\log(1-\nabla)}\cdot\frac{(1-\nabla)}{\nabla} f_0.$$

Multiplying through by ∇^2

$$\nabla^2 y_m = \left\{\frac{h}{\frac{\log(1-\nabla)}{\nabla}}\right\}^2 f_m + h(\nabla-\nabla^2)\,y_0' + \frac{h}{\frac{\log(1-\nabla)}{\nabla}}\cdot(\nabla-\nabla^2) f_0 = \left\{\frac{h}{\frac{\log(1-\nabla)}{\nabla}}\right\}^2 f_m$$

since ∇ operating on a constant yields zero.

For simplicity of notation we let $z_i = \nabla^2 y_i$ and write

$$z_i = \left\{\frac{h}{\frac{\log(1-\nabla)}{\nabla}}\right\}^2 f_i \qquad (1)$$

Let $a_0 + a_1\nabla + a_2\nabla^2 + \dots$ be the power series expansion of $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$. The power series can be approximated by a rational fraction by use of the following technique. $a_0 + a_1\nabla + a_2\nabla^2 + \dots + a_n\nabla^n \simeq \frac{b_0 + b_1\nabla + b_2\nabla^2 + \dots + b_q\nabla^q}{1 + c_1\nabla + c_2\nabla^2 + \dots + c_p\nabla^p}$. Multiplying each side by the denominator of the above fraction and equating coefficients of the like power terms in ∇ we generate p+q+1 linear equations in the p+q+1 unknowns $b_0 \dots b_q$, $c \dots c_p$.

$$\begin{aligned}
b_0 &= a_0\\
b_1 &= a_1 + a_0c_1\\
b_2 &= a_2 + a_1c_1 + a_0c_2\\
b_3 &= a_3 + a_2c_1 + a_1c_2 + a_0c_3\\
&\;\vdots \qquad\quad \vdots
\end{aligned}$$

The solution of this system gives us the coefficients of the rational fraction which agrees with the series out to p+q+1 terms.

It should be noted that a given polynomial of degree r can be equated

identically to each of r + 1 distinct functions. Truncating the polynomial after 1, 2, ..., n terms, successively, we obtain a collection of polynomial fractions which can be arranged as a Padé table of rational convergents. Fig. 1 is the Padé table associated with $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$, where a third degree polynomial is used to generate the rational convergents.

The power series expansion of $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$, truncated to seven terms, is the sixth degree polynomial

$$1+\nabla+\frac{11}{12}\nabla^2+\frac{5}{6}\nabla^3+\frac{137}{180}\nabla^4+\frac{7}{10}\nabla^5+\frac{363}{560}\nabla^6. \qquad (3)$$

The coefficients of this polynomial were used as inputs to Program E UCSD PADÉ (Naval Postgraduate School Library Routine) to obtain coefficients of the 26 Padé convergents whose numerators and denominators are polynomials of degree q and p, respectively, and where p+q ≤ 6. Fig. 2 lists these coefficients, rounded to three significant figures.

As stated above, each of these convergents is identically equal to (3) out to p+q+1 terms. Moreover, a given convergent expanded algebraically into a power series generally continues to agree quite well with the related infinite series for a number of terms beyond the (p+q+1)st; i.e., a rational convergent generally is a better approximation to a function than is the truncated series from which the convergent was derived.

Designate a particular convergent to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ by

$$\frac{AN(1)+AN(2)\nabla+AN(3)\nabla^2+\cdots+AN(q+1)\nabla^q}{AD(1)+AD(2)\nabla+AD(3)\nabla^2+\cdots+AD(p+1)\nabla^p}. \qquad (4)$$

Suppose we wish to find an approximate numerical solution of the equation $y'' = f(x,y)$. Substituting (4) for $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ in equation (2) we have

$$\delta_i = h^2 f_i \Big/ \left(\frac{AN(1)+\cdots+AN(q+1)\nabla^q}{AD(1)+\cdots+AD(p+1)\nabla^p}\right).$$

Rewritten, this becomes $(AN(1)+\cdots+AN(q+1)\nabla^q)\delta_i = h^2(AD(1)+\cdots+AD(p+1)\nabla^p)f_i$.

Noting that [illegible], we can express the above equation in the form [illegible] (5)

Denote the coefficients in (5) as follows:

$$Q(j) = \sum_{i=j}^{q} \binom{i}{j} Ab(i+1)$$

$$P(j) = \sum_{i=j}^{p} \binom{i}{j} Aa(i+1)$$

Substituting the coefficients in (5) we have:

$$Q(0)z_i - Q(1)z_{i-1} + \dots \pm Q(q)z_{i-q} = h^2\left[P(0)f_i - P(1)f_{i-1} + \dots \pm P(p)f_{i-p}\right], \text{ or,}$$

$$z_i = \frac{1}{Q(0)}\left\{Q(1)z_{i-1} - \dots \mp Q(q)z_{i-q} + h^2\left[P(0)f_i - \dots \pm P(p)f_{i-p}\right]\right\}. \qquad (6)$$

Here z_i is given in terms of coefficients of the Padé convergent and of previously computed values of z and f. Recalling that $z_i = \nabla^2 y_i = y_i - 2y_{i-1} + y_{i-2}$ we may now calculate $y_i = z_i + 2y_{i-1} - y_{i-2}$. The value of f_i used in (6) will have been computed from a first approximation to y_i generated by a predictor formula.

3. Stability Considerations.

The recursion formula generated from a given Padé convergent is of the form: $Q(0)z_i = Q(1)z_{i-1} - \dots \pm Q(q)z_{i-q} + h^2\left[P(0)f_i - \dots \pm P(p)f_{i-p}\right]$, (7)

where Q(i) and P(i) are as defined in Section 2.

Substituting $\nabla^2 y_i = y_i - 2y_{i-1} + y_{i-2}$ for z_i in (7) we obtain

$$Q(0)\,(y_i - 2y_{i-1} + y_{i-2}) = Q(1)\,(y_{i-1} - 2y_{i-2} + y_{i-3}) - \dots \pm Q(q)\,(y_{i-q} - 2y_{i-q-1} + y_{i-q-2}) = h^2\left[P(0)f_i - P(1)f_{i-1} + \dots \pm P(p)f_{i-p}\right]$$

Multiplying and collecting terms, this becomes

$$\begin{aligned} Q(0)y_i &= \left[Q(1) + 2Q(0)\right]y_{i-1} - \left[Q(2) + 2Q(1) + Q(0)\right]y_{i-2} + \dots \\ &+ (-1)^{q+1}\left[Q(q) + 2Q(q-1) + Q(q-2)\right]y_{i-q} + (-1)^{q}\left[2Q(q) + Q(q-1)\right]y_{i-q-1} \\ &+ (-1)^{q-1}Q(q)y_{i-q-2} + h^2\left[P(0)f_i - \dots + (-1)^{p}P(p)f_{i-p}\right] \end{aligned} \qquad (8)$$

The general solution of this difference equation is of the form

$y_n = c_1 r_1^n + c_2 r_2^n + \dots + c_n r_n^n$ where $r_1, r_2, \dots, r_n$ are roots of the associated characteristic equation (to be introduced later) and the c_i are constants.

Consider the 2nd order Padé convergent $\frac{1}{1-\sigma+\frac{1}{12}\sigma^2}$ (Formula 1) in Fig. 1). From the discussion of Section 2 we know that the recursion formula generated by this convergent will have the following coefficients:

$$Q(0) = 1; \quad Q(i) = 0, \; i \geq 1$$

$$P(0) = \tfrac{1}{12}; \; P(1) = -\tfrac{10}{12}; \; P(2) = \tfrac{1}{12}; \; P(i) = 0, \; i \geq 3$$

The general recursion formula (8) then becomes

$$y_i = 2y_{i-1} - y_{i-2} + h^2\left[\tfrac{1}{12} f_i + \tfrac{10}{12} f_{i-1} + \tfrac{1}{12} f_{i-2}\right]. \qquad (9)$$

In the initial value problem (1) it is seen that $f_i = -y_i$. Substituting in (9) and collecting terms:

$$(1 + \tfrac{1}{12}h^2)y_i = (2 - \tfrac{10}{12}h^2)y_{i-1} - (1 + \tfrac{1}{12}h^2)y_{i-2}$$

or,

$$(12+h^2)y_i - (24-10h^2)y_{i-1} + (12+h^2)y_{i-2} = 0$$

Finding roots:

$$r = \frac{(24-10h^2) \pm \sqrt{(24-10h^2)^2 - 4(12+h^2)^2}}{2(12+h^2)}$$

$$= \frac{(12-5h^2) \pm ih\sqrt{144-24h^2}}{12+h^2} \qquad (10)$$

Ignoring terms of the order of h^2 we have

$$r \simeq \frac{12 \pm 12hi}{12} = 1 \pm ih \qquad (11)$$

The general solution of (9) is of the form

$$y_n = c_1 r_1^n + c_2 r_2^n$$

We determine the coefficients c_i from the solution $y = \cos x$ of the initial value problem.

$y_0 = c_1 r_1^0 + c_2 r_2^0 = 1$ (initial conditions give $y_0 = 1$)

$y_1 = c_1 r_1 + c_2 r_2^1 = 1 - \frac{h^2}{2}$ ($y = \cos h = 1 - \frac{h^2}{2} + \frac{h^4}{4!} \dots$. For small values of h, $1 - \frac{h^2}{2}$ is a good approximation)

Solving these equations simultaneously:

$$c_1 = \frac{2i-h}{4i} \quad , \quad c_2 = \frac{2i+h}{4i}$$

Thus we have:

$$y_n = \frac{2i-h}{4i}(1+hi)^n + \frac{2i+h}{4i}(1-hi)^n \qquad (12)$$

This can be written in trigonometric form:

$$y_n = \left(\tfrac{1}{2}+\tfrac{h}{4}i\right)\left[\left(\sqrt{1+h^2}\right)^n(\cos\theta+i\sin\theta)^n\right] + \left(\tfrac{1}{2}-\tfrac{h}{4}i\right)\left[\left(\sqrt{1+h^2}\right)^n(\cos\theta-i\sin\theta)^n\right]$$

where $\theta = \text{arc}\sin\frac{h}{\sqrt{1+h^2}}$.

$$y_n = \left(\sqrt{1+h^2}\right)^n\left\{\left(\tfrac{1}{2}+\tfrac{h}{4}i\right)(\cos n\theta+i\sin n\theta) + \left(\tfrac{1}{2}-\tfrac{h}{4}i\right)(\cos n\theta - i\sin n\theta)\right\}$$

$$= \left(\sqrt{1+h^2}\right)^n\left(\cos n\theta - \frac{h}{2}\sin n\theta\right) \qquad (13)$$

for small h, $h \simeq \theta$, in which case

$$y_n \simeq \left(\sqrt{1+h^2}\right)^n\left(\cos nh - \frac{h}{2}\sin nh\right)$$

and this solution converges to the exact solution.

It can be seen from the graphs that Formulas 10, 11, 12, 15, 23, and 25 are the most promising from the standpoint of minimum error amplification. Unfortunately, their associated characteristic equations (fourth through seventh degree) are too intractable to permit analysis. It would be quite simple, however, to obtain the roots of these equations with an appropriate computer program. The error characteristics of the equations could then be determined from a study of the properties of their roots. This is discussed in Section 7 as a project recommended for future study.

The foregoing paragraphs were concerned with the accumulation of truncation error without regard for the fact that errors in y_n and y_{n-1} in (5) will affect subsequent errors. To consider this effect a different approach will be taken.

In terms of the difference equation (9),

$$\bar{y}_i = 2\bar{y}_{i-1} - \bar{y}_{i-2} + h^2\left[\frac{1}{12}\bar{f}_i + \frac{10}{12}\bar{f}_{i-1} + \frac{1}{12}\bar{f}_{i-2}\right] + T(h) + R(i) \qquad (14)$$

where $\bar{y}_i$ is the value of solution of the initial value problem at x_i, and $\bar{f}_i = f(x_i, \bar{y}_i)$. T(h) is the truncation error introduced by using $\frac{1}{1+\frac{1}{12}\delta^2}$ to approximate $\left\{\frac{\log(1+\Delta)}{\Delta}\right\}^2$, and R(i) is the roundoff error. We define E(h,i) = T(h) + R(i).

Defining $\epsilon_i = \bar{y}_i - y_i$, we subtract (9) from (14) and obtain

$$\epsilon_i = 2\epsilon_{i-1} - \epsilon_{i-2} + h^2\left[\frac{1}{12}(\bar{f}_i - f_i) + \frac{10}{12}(\bar{f}_{i-1} - f_{i-1}) + \frac{1}{12}(\bar{f}_{i-2} - f_{i-2})\right] + E(h,i).$$

Assuming that $f_i(x_i, y)$ is differentiable with respect to y in the interval $(\bar{y}_i, y_i)$ we may use the mean value theorem to write:

$$(\bar{f}_i - f_i) = f_y(x_i, \xi_i)(\bar{y}_i - y_i) = \epsilon_i f_y(x_i, \xi_i).$$

If $f_y(x_i, \xi_i)$ does not vary greatly we may let $f_y(x_i, \xi_i) = K$ and write

$$\epsilon_i = 2\epsilon_{i-1} - \epsilon_{i-2} + h^2K\left[\frac{1}{12}\epsilon_i + \frac{10}{12}\epsilon_{i-1} + \frac{1}{12}\epsilon_{i-2}\right] + E(h,i).$$

Collecting terms: $(1 - \frac{1}{12}h^2K)\epsilon_i = (2 + \frac{10}{12}h^2K)\epsilon_{i-1} - (1 - \frac{1}{12}h^2K)\epsilon_{i-2} + E(i,h)$

or, $(12 - h^2K)\epsilon_i = (24 + 10h^2K)\epsilon_{i-1} - (12 - h^2K)\epsilon_{i-2} + E(i,h)$.

In the solution of the initial value problem (1), $K = f_y(x_i, \xi_i) = -1$. Hence, $(12+h^2)\epsilon_i = (24-10h^2)\epsilon_{i-1} - (12+h^2)\epsilon_{i-2} + E(h,i)$. (15)

Under the assumption that E(h,i) is relatively insensitive with respect to i, we may proceed as we did in solving (9). (As applied to this case the truncation error $T(h) = Ch^4y^{(4)}(\xi_i)$, and $y^{(4)}(\xi_i)$ varies slowly when the h increments are small). We will henceforth assume E(h,i) to be a constant: Dh^4.

We must solve $(12 + h^2)\epsilon_i = (24-10h^2)\epsilon_{i-1} - (12+h^2)\epsilon_{i-2} + Dh^4$
$\epsilon_0 = 0$ (no error initially), and
$\epsilon_1 = \delta$ (assumed to be non-zero)

The solution consists of the general solution corresponding to the homogeneous part $\epsilon_i = c_1r_1^i + c_2r_2^i$ and a particular solution there-

ponding to the non-homogeneous part Dh^4. The particular solution can be found by assuming that ϵ_n is a constant A, so that

$$(12+h^2)A = (24-10h^2)A - (12+h^2)A + Dh^4. \text{ Hence,}$$

$$A = \frac{Dh^4}{2(12+h^2)-(24-10h^2)} = \frac{Dh^4}{12h^2} = \frac{Dh^2}{12}.$$

The complete solution is then $\epsilon_n = c_1 r_1^n + c_2 r_2^n + \frac{D}{12}h^2$. (16)

Let $r_1 = a + ib$, $r_2 = a - ib$.

Denote $c_1 = \alpha + i\beta$, $c_2 = \alpha - i\beta$, where $\alpha = -\frac{D}{24}h^2$ and $\beta = -\frac{1}{2b}\left\{\delta + (a-1)\frac{D}{12}h^2\right\}$.

The solution (16) is transformed into trigonometric form by letting

$$\theta = \text{arc sin } \frac{b}{\sqrt{a^2+b^2}}$$

Then, $\epsilon_n = |r|^n (2\alpha \cos n\theta - 2\beta \sin n\theta) + \frac{D}{12}h^2$. Expanding:

$$\epsilon_n = |r|^n \left\{-\frac{D}{12}h^2 \cos n\theta + \frac{1}{b}\left(\delta + (a-1)\frac{D}{12}h^2\right) \sin n\theta\right\} + \frac{D}{12}h^2.$$

In particular, if we approximate

$a = 1$ $b = h$, i.e., $r_1 = 1 + ih$, $r_2 = 1 - ih$

$$\epsilon_n = (\sqrt{1+h^2})^n \left\{-\frac{D}{12}h^2 \cos n\theta + \frac{1}{h}(\delta \sin n\theta)\right\} + \frac{D}{12}h^2 \quad (17)$$

where $\theta = \text{arc sin } \frac{h}{\sqrt{1+h^2}}$. For small h

$$\epsilon_n \simeq (\sqrt{1+h^2})^n \left\{-\frac{D}{12}h^2 \cos nh + \frac{\delta}{h} \sin nh\right\} + \frac{D}{12}h^2. \quad (18)$$

This solution of the error propagation equation qualitatively explains the behavior of the experimental results displayed in Fig. 16.

a. If h is small, the sine term of $\left\{-\frac{D}{12}h^2 \cos nh + \frac{\delta}{h} \sin nh\right\}$ is significant and the cosine term is negligible. Error would be expected to vary nearly sinusoidally.

b. ϵ_n should be approximately equal to zero where nh is multiple of π, since the term $\frac{\delta}{h}$ sin nh will vanish at these points. Given h = .02 and solving for $n = \frac{k\pi}{.02}$, k = 1, 2, ..., 5, we expect to find

near-zero error where n = 157, 314, 471, 628 and 785. Fig. 16 shows this to be the case. Error nulls shown in Figs. 33 and 41 can be explained similarly by solving for n with h = .01 and .05, respectively.

c. The bracketed term in (18) is multiplied by $|r|^n$. Hence, the error magnitude should grow with increasing n if $|r| > 1$ and diminish if $|r| < 1$. The amplification factor $(\sqrt{1+h^2})^n$ in (18) is only an approximation of $|r|^n$. The actual roots were found to be

$$r = \frac{(12-5h^2) \pm ih\sqrt{144-24h^2}}{12+h^2}$$

$$|r|^2 = \frac{(144-120h^2+25h^4)+h^2(144-24h^2)}{144+24h^2+h^4} = 1$$

for all h. Whenever h is small enough to insure that (18) closely approximates (17), error maxima should remain nearly constant. Fig. 33 substantiates this for h = .01. Increasing error maxima in Figs. 19 and 41 (h = .02 and .05, respectively) are attributed to the failure of h to meet the criterion stated above.

No explanation is offered for the high frequency error oscillation so prevalent in some of the graphs, e.g. Fig. 16. Investigation of this phenomenon is suggested as a project for future study.

4. Description of the Test Program.

This program is designed to solve a given second order differential equation 26 times, successively using each of 26 Padé convergents to generate a central recursion formula. Integration of the given equation is by the predictor-corrector method, using the Milne predictor formula: $y_n = y_{n-1} + y_{n-3} - y_{n-4} + \frac{h^2}{4}\left[5y''_{n-1} + 2y''_{n-2} + 5y''_{n-3}\right]$. Necessary starting values are computed by the Runge-Kutta method. The iterative process may be carried out to as many as 900 steps, solution error being

determined at each step if an exact solution of the given equation is known. Graphs are plotted with error as ordinate and number of iterations as abscissa. Fig. 3 explains the symbols used in the program. Fig. 4 is a printout of the program used to evaluate the equation generating the cosine function, y" + y = 0 (Program TMOD 2). Fig. 5 is a printout of the program used to evaluate the Coulomb Wave Equation $y'' + y\left(1 - \frac{2\eta}{x} - \frac{L(L+1)}{x^2}\right) = 0$ (Program TMOD 6).

5. Discussion of Data.

a. Program TMOD 2

(1) Figs. 7 through 25 are graphs of progressive error resulting when the initial value problem y" + y = 0, y(0) = 1, y'(0) = 0 is solved using an integration step length of .02 and corrector formulas derived from the various Padé convergents. Fig. 6 relates the recursion formula number shown on each graph to a description of the corresponding Padé fraction. Formulas 16, 17, 20, 21, 23, 24 and 26 diverged rapidly and no associated graphs were plotted.

(a) Formulas 10, 11, 12, 15, 22 and 25 produced remarkable accuracy over the entire range of 900 iterations.

(b) Formula 6 (Fig. 12), although less accurate than the group just discussed, has an important property: error maxima are diminished with increasing iteration.

(c) The remaining graphs indicate that error maxima are not being damped but are increasing linearly with respect to n, the number of iterations.

(2) The next set of data was obtained by repeating the preceding experiment after decreasing the integration step length to .01.

The following were observed:

(a) The runs which proved to be most accurate with a step length of .02 (Formulas 10, 11, 12, 15, 22 and 25) were found to be less accurate with the smaller step length (contrary to what would be expected). Formulas 15, 22 and 25 show a small error amplification while all the others in this group show a much greater error amplification. Figs. 28 through 33 are graphs showing these results.

(b) Formula 6 provides less accurate results than with the greater step length but its error damping characteristics remain. (Fig. 27)

(c) Formula 5 is more stable. Its accuracy is comparable to that in the preceding run. (Fig. 26)

(d) All other formulas proved to be more accurate than when used with the greater step length. All of them, however, amplify errors.

(e) The error graphs associated with Formulas 9, 10, 11, 13, 14, 18, 22 and 25 were identical. (Fig. 33)

(3) Increasing the step length to .05 had the following effects:

(a) The formulas which proved best with a step length of .02 are much less accurate with a step length of .05. Figs. 34 through 41 are the error graphs associated with Formulas 6, 10, 11, 12, 13, 15, 22 and 25 using the .05 step length. These graphs show the only formulas retaining any error damping characteristics to be numbers 11, 12 and 25.

b. Program [illegible] 6

(1) The Coulomb Wave Equation was solved for two combinations of values of L and η ($L=1, \eta=1$; and $L=2, \eta=3$), and with various integration step lengths. It was not feasible to generate error graphs for these equations. Fig. 42 lists magnitude of deviation of computed solutions from true values after the number of iterations indicated. The

to limitations of the tables used[5], the minimum error discernable was 1E-7 ($1 = 10^{-7}$). An examination of Fig. 42 reveals the following:

(a) Identical results were obtained in all cases where Formulas 9, 13, 14, 15 and 18 were used. This group also produced the most accurate solutions. Reducing step length improved accuracy throughout the range.

(b) Formula 8 solutions were slightly less accurate than those of the group above in solving the equation $y'' + y\,(1-\frac{2}{x}-\frac{2}{x^2}) = 0$. Solutions of the equation $y'' + y(1-\frac{6}{x}-\frac{6}{x^2}) = 0$, using a step length of .02 were more accurate than with any other formula.

6. Conclusions.

In his Numerical Methods[3], Kopal illustrated the shortcomings of going-ahead recursion formulas: those derived from the relationship $y_i = \left\{\frac{h}{\log E}\right\}^2 Ef_{i-1}$. When using going-across formulas stemming from the integration formula $y_i = \left\{\frac{h}{\log e}\right\}^2 f_i$, an approximation of f_i must be obtained before y_i can be calculated. Therefore, the method suggested by Kopal is essentially the predictor-corrector method coupled with a procedure for deriving an unlimited supply of corrector formulas. Some of these we have seen produce quite accurate solutions to several differential equations of second order. A glance at Figs. 43 - 45, the error of $y'' + y = 0$ after solution by the Milne method, is evidence of the superiority of a number of the correctors derived from Padé convergents.

It is suggested at this point that the less accurate going-ahead type formulas might be generated in the same way and used as predictors.

The fact that certain correctors derived from Padé counterparts perform their tasks so well should provide sufficient motivation for a similar study of predictor derivation.

None of the corrector formulas discussed in this paper are stable for all equations over all ranges of h. Additional formulas could be derived from a polynomial approximation to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ of higher degree, but this area does not appear promising. In dealing with associated characteristic equations of higher degree it will be extremely difficult to locate values of parameters which will retain all roots within the required bounds.

The excellent results obtained with Formula 15 (Fig. 21) indicate that a fourth degree polynomial approximation to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ is sufficient to insure that truncation error is not a significant problem. It would seem, therefore, that the use of polynomials of higher degree would invite additional stability complications.

In summary, it is concluded that the procedure suggested by [illegible] should be viewed as a method of deriving predictor and corrector formulas. The results achieved with some of the correctors derived in this manner indicate that this procedure is promising and merits further study.

7. Recommendations for Future Studies.

a. Investigate the roots of the characteristic equations associated with the more promising recursion formulas discussed in this paper. Ascertain and tabulate values of $\bar{h}$ for which all roots lie within the unit circle. With this data available, one could readily select the best recursion formula for solving a given differential equation over a

specified range of values of the independent variable.

b. Derive a Padé table of rational convergents to [illegible] from which to obtain a number of going-ahead recursion formulas. Substitute each of these in turn for the predictor formula used in Program [illegible] 5. Calculate errors and compare with Fig. 42. In this manner, evaluate the merits of predictor formulas derived from rational Padé convergents. Ralston [6] describes the advantages of using predictors and correctors of the same order.

c. Extend the polynomial representation of [illegible] beyond seven terms and derive higher order recursion formulas. Investigate the roots of these formulas as suggested in subparagraph a above.

specified range of values of the independent variable.

b. Derive a Padé table of rational convergents to [illegible] from which to obtain a number of going-ahead recursion formulas. Substitute each of these in turn for the predictor formula used in Program [illegible] 6. Calculate errors and compare with Fig. 32. In this manner, evaluate the merits of predictor formulas derived from rational Padé convergents. Ralston [illegible] describes the advantages of using predictors and correctors of the same order.

c. Extend the polynomial representation of [illegible] beyond seven terms and derive higher order recursion formulas. Investigate the roots of these formulas as suggested in subparagraph a above.

Fig. 1 - Sample Padé Table

p \ q	0	1	2	3
0	$\frac{1}{1}$	$\frac{1+\nabla}{1}$	$\frac{1+\nabla+\frac{11}{12}\nabla^2}{1}$	$\frac{1+\nabla+\frac{11}{12}\nabla^2+\frac{5}{6}\nabla^3}{1}$
1	$\frac{1}{1-\nabla}$	$\frac{1+\frac{1}{12}\nabla}{1-\frac{11}{12}\nabla}$	$\frac{1+\frac{1}{11}\nabla+\frac{1}{132}\nabla^2}{1-\frac{10}{11}\nabla}$	
2	$\frac{1}{1-\nabla+\frac{1}{12}\nabla^2}$	$\frac{1}{1-\nabla+\frac{1}{12}\nabla^2}$		
3	$\frac{1}{1-\nabla+\frac{1}{12}\nabla^2}$			

Convergents to $\left\{\frac{\log(1-\nabla)}{\nabla}\right\}^2$ derived from third degree polynomial.

The fact that three of these convergents are equal is coincidental.

Fig. 2 - Coefficients of Padé Convergents to $\left\{ \frac{\log(1-x)}{x} \right\}^2$

No.	Numerator	Denominator
1	1.0	1.0
2	1.0,1.0	1.0
3	1.0,1.0,.917	1.0
4	1.0,1.0,.917,.833	1.0
5	1.0,1.0,.917,.833,.761	1.0
6	1.0,1.0,.917,.833,.761,.700	1.0
7	1.0	1.0,-1.0
8	1.0,.083	1.0,-.917
9	1.0,.091,.008	1.0,-.909
10	1.0,.087,.003,-.004	1.0,-.913
11	1.0,.080,-.003,-.010,-.005	1.0,-.920
12	1.0,.074,-.009,-.016,-.011,-.005	1.0,-.926
13	1.0	1.0,-1.0,.083
14	1.0,0.0	1.0,-1.0,.083
15	1.0,.600,.050	1.0,-.400,-.500
16	1.0,-1.29,-.121,-.014	1.0,-2.29,1.25
17	1.0,-.830,-.082,-.013,-.002	1.0,-1.83,.832
18	1.0	1.0,-1.0,.083
19	1.0,.083	1.0,-.917,.003,.004
20	1.0,-1.0,.050	1.0,-2.0,1.13,-.133
21	1.0,-.954,.077,.002	1.0,-1.95,1.12,-.155
22	1.0	1.0,-1.0,.083,0.0,-.004
23	1.0,-1.0	1.0,-2.0,1.08,-.083,-.004
24	1.0,-1.0,.123	1.0,-2.0,1.21,-.[illegible],.00[illegible]
25	1.0	1.0,-1.0,.083,0.0,-.004,-.[illegible]
26	1.0,-.877	1.0,-1.[illegible],.960,-.073,-.00[illegible],-.00[illegible]

Fig. 3 - Legend of Program Symbols

X	Independent variable
Y	Dependent variable
YP	y'
YDP	y''
YT	$\bar{y}$
ERROR	$\bar{y} - y$
D(I)	∇y
Z(I)	$\nabla^2 y$
AN(2)	Coefficient of 2nd numerator term in Padé convergent
AD(4)	Coefficient of 4th denominator term in Padé convergent
AX, AY, AYP, AYDP	Initial values
JP	Number of first convergent to be evaluated (1≤JP≤[illegible])
JQ	Number of last convergent to be evaluated (1≤JP≤JQ≤[illegible])
H	h (integration step length)
N	Number of starting values to be computed by Runge-Kutta method
M	Total number of iterations desired
IN(I)	Denotes number of terms in numerator of formula no. (I). Used for information in printout
ID(I)	Same as IN(I), except refers to denominator terms
DEL(K,I,J)	Array which stores Padé coefficients. K=1 denotes numerator coefficient; K=2, denominator coefficient. I is index no. of convergent. J is the number of a specific term. E.g., DEL(2,7,4) denotes the coefficient of the fourth term in the denominator of convergent no.7.
Q0	Coefficient of y_i in recursion formula
Q(J)	Coefficient of y_{i-j} in recursion formula
P0	Coefficient of y''_i in recursion formula
P(J)	Coefficient of y''_{i-j} in recursion formula
L	Index no. of convergent and its associated recursion formula

Fig. [illegible] - Program [illegible] (Printout)

```
      [illegible]
C
      [illegible]
     1      [illegible]
     2      [illegible]
  [illegible] FORMAT [illegible]
  [illegible] FORMAT [illegible]
  [illegible] FORMAT [illegible]
  [illegible] FORMAT [illegible]
  [illegible] FORMAT [illegible]
  [illegible] FORMAT [illegible]
C
C     [illegible]
      [illegible]
      [illegible]
      [illegible]
      DO [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
C
C     [illegible]
      DO [illegible]
      DO 701 [illegible]
      [illegible]
  701 CONTINUE
C
C     [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      DO [illegible]
      [illegible]
      [illegible]
   [illegible]
      [illegible]
  [illegible]
  [illegible]
      [illegible]
      [illegible]
   [illegible] CONTINUE
      [illegible]
      [illegible]
  [illegible]
      [illegible]
      [illegible]
      [illegible]
  [illegible]
```

Fig. 4 (cont'd)

```
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
  100 CONTINUE
*
C     COMPUTE FIRST AND SECOND DIFFERENCES OF Y
      DO 61 I=2,N
   61 D(I)=Y(I)-Y(I-1)
      DO 92 I=3,N
   92 Z(I)=D(I)-D(I-1)
*
C     SELECT PADE CONVERGENT TO BE USED
      L=JP
*
C     COMPUTE COEFFICIENTS OF RECURSION FORMULA FROM
C     COEFFICIENTS OF PADE CONVERGENT
      AN(1)=1.0
      AD(1)=1.0
  206 CONTINUE
      DO 207 J=2,6
      AN(J)=DEL(1,L,J)
  207 AD(J)=DEL(2,L,J)
   12 QQ=0.0
  203 PQ=0.0
      DO 14 J=1,6
  202 QQ=QQ+AN(J)
   14 PQ=PQ+AD(J)
      DO 15 J=1,5
      Q(J)=0.0
      P(J)=0.0
      DO 15 I=J,5
      Q(J)=Q(J)+AN(I+1)*BINOM(I,J)
   15 P(J)=P(J)+AD(I+1)*BINOM(I,J)
*
      NN=N+1
      DO 1[illegible] I=NN,M
*
C     COMPUTE APPROXIMATE VALUE OF Y WITH MILNE PREDICTOR
      Y(I)=Y(I-1)+Y(I-3)-Y(I-4)+(H**2/4.0)*(5.0*YPP(I-1)
     1     +2.*YPP(I-2)+5.*YPP(I-3))
      YPP(I)=-Y(I)
*
C     USE RECURSION FORMULA DERIVED FROM PADE CONVERGENTS
C     TO COMPUTE SECOND DIFFERENCES OF Y
      QQ=-Q(1)*Z(I-1)+Q(2)*Z(I-2)-Q(3)*Z(I-3)+Q(4)
     1     *Z(I-4)-Q(5)*Z(I-5)
      PP=(PQ*YPP(I)-P(1)*YPP(I-1)+P(2)*YPP(I-2)-P(3)
     1     *YPP(I-3)+P(4)*YPP(I-4)-P(5)*YPP(I-5))*(H**2)
      Z(I)=(PP-QQ)/QQ
```

Fig. 4 (cont'd)

```
*
C     CALCULATE Y FROM SECOND DIFFERENCE JUST COMPUTED
      D(I)=D2(I)+D(I-1)
      Y(I)=D(I)+Y(I-1)
   19 YDP(I)=-Y(I)
*
C     COMPUTE TRUE VALUES OF Y AND CALCULATE ERROR
  210 DO 20 I=1,M
      XI(I)=I
      AI=I
      YT(I)=COSF(H*AI)
   20 ERROR(I)=Y(I)-YT(I)
*
      LABEL=IBCD(L,0,4,IER)
      CALL DRAW (M,XI,ERROR,0,0,LABEL,ITITLE,0.,0.,0,0,0,0,
     1     5,5,1,LAST)
      IF (L-10) 24,25,25
   24 L=L+1
      GO TO 206
   25 PRINT 999
      END
      FUNCTION BINOM (M,N)
      AM=M
      IF (N-0)301,302,302
  302 IF (N-1)303,304,305
  305 IF (M-N)301,303,306
  306 CONTINUE
      K=N-1
      NUM=M
      NDNOM=N
      DO 444 I=1,K
      NUM=NUM*(M-I)
  444 NDNOM=NDNOM*(N-I)
      XNUM=NUM
      XD=NDNOM
      BINOM=XNUM/XD
      GO TO 999
  303 BINOM=1.0
      GO TO 999
  304 BINOM=AM
      GO TO 999
  301 PRINT 312
  312 FORMAT (18H BINOM INPUT FAULT)
  999 END
```

Fig. 5 – Program [illegible] G (Continued)

```
      [illegible]
      DIMENSION [illegible]
     1     [illegible]
     2      [illegible]

 1000 FORMAT [illegible]
 1001 FORMAT [illegible]
 1002 FORMAT (F1[illegible].6,1PE15.7,[illegible],1PE1[illegible].7)
 1003 FORMAT (4H1 H=,F8.3,4H  M=,I4,4H  N=,I4,5H ETA=,F8.3,
     1       4H L=,F4.1//)
 1004 FORMAT (I1,I2,2I1,1P4E16.10)
 1005 FORMAT (13H FORMULA NO. ,I2,8H.  NUM =,I3,
     1      8H  DENOM =,I3//)
 1006 FORMAT (1P4E20.7)
 1007 FORMAT (15H  JOB COMPLETED)
C
C     READ INPUT DATA
      READ 1000, NF, JN
      READ 1001,H,N,M,IS,IT
      READ 1002, AX,AY,AYP,ETA,ZL,CO
      PRINT 1003, H,N,M,ETA,ZL
C
C     CONVERT INITIAL VALUES FROM NORMALIZED
C     FORM USED IN MOST TABLES INTO STANDARD FORM
C     DESCRIBED IN THIS PROGRAM AS Y
      LL=ZL
      CL=CO
      DO 201 L=1,LL
  201 CL=(ZL*SQRTF(ZL**2+ETA**2))/(ZL*(2.*ZL+1.))
      AY=AY*CL*(AX**(LL+1))
      A(LL+1)=1.
      A(LL+2)=ETA/(ZL+1.)
      JL=LL+3
      DO 202 L=JL,100
      XL=L
  202 A(L)=(2.*ETA*A(L-1)-A(L-2))/((XL+ZL)*(XL-ZL-1.))
      PHIS=0.0
      JL=LL+1
      DO 203 L=JL,100
      XL=L
  203 PHIS=PHIS+XL*A(L)*AX**(L-LL-1)
      AYP=CL*PHIS*(AX**LL)
C
C     READ PADE COEFFICIENTS
      DO 11 K=1,32
   11 READ 1004, K,I,(N(I),ID(I),(AML(K,I,J),J=2,6))
C
C     COMPUTE N STARTING VALUES BY RUNGE KUTTA METHOD
      V=AAYP
      X(IS)=AX
      Y(IS)=AY
      YP(IS)=AYP
      YPP(IS)=-AY*(1.-(2.*ETA)/AX-(ZL*(ZL+1.))/AX**2)
      IS1=IS+1
      IS2=IS+2
      DO 103 I=IS1,N
```

Fig. 3 (cont'd)

```
      DO 104 J=1,4
      GO TO (100,101,101,102),J
  100 XX=X(I-1)
      YY=Y(I-1)
      GO TO 103
  101 XX=X(I-1)+H/2.
      YY=Y(I-1)+V/2.+DK(1)/8.
      GO TO 103
  102 XX=X(I-1)+H
      YY=Y(I-1)+V+DK(3)
  103 YYDP=-YY*(1.-(2.*ETA)/XX-(ZL*(ZL+1.))/XX**2)
  104 DK(J)=(H**2/2.)*YYDP
      DKT=(DK(1)+DK(2)+DK(3))/3.
      DKP=(DK(1)+2.*DK(2)+2.*DK(3)+DK(4))/3.
      X(I)=X(I-1)+H
      Y(I)=Y(I-1)+V+DKT
      V=V+DKP
      YP(I)=V/H
  105 YDP(I)=-Y(I)*(1.-(2.*ETA)/X(I)-(ZL*(ZL+1.))/X(I)**2)
*
C     COMPUTE FIRST AND SECOND DIFFERENCES OF Y
      DO 106 I=IS1,N
  106 D(I)=Y(I)-Y(I-1)
      DO 107 I=IS2,N
  107 E(I)=D(I)-D(I-1)
*
C     SELECT PADE CONVERGENT TO BE USED
      L=JP
*
C     COMPUTE RECURSION FORMULA COEFFICIENTS FROM PADE
C     COEFFICIENTS
      AN(1)=1.0
      AD(1)=1.0
  108 CONTINUE
      DO 109  J=2,6
      AN(J)=DEL(1,L,J)
  109 AD(J)=DEL(2,L,J)
      QQ=0.0
      PQ=0.0
      DO 110 J=1,6
      QQ=QQ+AN(J)
  110 PQ=PQ+AD(J)
      DO 111 J=1,5
      Q(J)=0.0
      P(J)=0.0
      DO 111 I=J,5
      Q(J)=Q(J)+AN(I+1)*BINOM(I,J)
  111 P(J)=P(J)+AD(I+1)*BINOM(I,J)
*
      NN=N+1
      DO 112 I=NN,M
      X(I)=X(I-1)+H
*
C     OBTAIN FIRST APPROXIMATION TO Y  BY USING MILNE PREDICTOR
```

Fig. 5 (cont'd)

```
      [illegible]
     1     [illegible]
      [illegible]
C
C     OBTAIN CORRECTED VALUE OF SECOND DIFFERENCE OF Y
C     USING FORMULA GENERATED FROM [illegible]
      [illegible]
     1     [illegible]
      [illegible]
     1     [illegible]
      [illegible]
C
C     COMPUTE Y FROM DIFFERENCES JUST CALCULATED
      D(I)=Z(I)+D(I-1)
      Y(I)=D(I)+Y(I-1)
  111 YDD(I)=-Y(I)*(1.-(2.*E/A)/X(I)-(ZL*(ZL+1.))/X(I)**2)
C
C     CONVERT ALL COMPUTED VALUES OF Y INTO
C     NORMALIZED FORM FOR COMPARISON WITH STANDARD TABLES
      DO 200 I=NN,M
  200 Y(I)=Y(I)/((ZL*(Y [illegible])**(ZL+1.)))
      PRINT 1005,L,(IN(L),IQ(L))
      PRINT 1006,(Y(I),I=15,M,IT)
      IF(L-JQ) 113,114,114
  113 L=L+1
      GO TO 108
  114 PRINT 1007
      END
      FUNCTION BINOM (M,N)
      AM=M
      IF(N-M)307,301,301
  301 IF (N-1)305,305,302
  302 IF (M-N)307,305,303
  303 K=N-1
      NUM=M
      NDNOM=N
      DO 304 I=1,K
      NUM=NUM*(M-I)
  304 NDNOM=NDNOM*(N-I)
      XNUM=NUM
      XD=NDNOM
      BINOM=XNUM/XD
      GO TO 308
  305 BINOM=1.
      GO TO 308
  306 BINOM=AM
      GO TO 308
  307 PRINT 3000
 3000 FORMAT (13H BINOM INPUT FAULT)
      STOP
  308 END
```

Fig. 5 - Relation of Formula Numbers to Pade Convergents

Formula	Degree of Convergent (N/D)	Formula	Degree of Convergent (N/D)
1	0/0	14	1/2
2	1/0	15	2/2
3	2/0	16	3/2
4	3/0	17	4/2
5	4/0	18	0/3
6	5/0	19	1/3
7	0/1	20	2/3
8	1/1	21	3/3
9	2/1	22	0/4
10	3/1	23	1/4
11	4/1	24	2/4
12	5/1	25	0/5
13	0/2	26	1/5

Fig. 7 - Formula 1 Error
Step length = .02

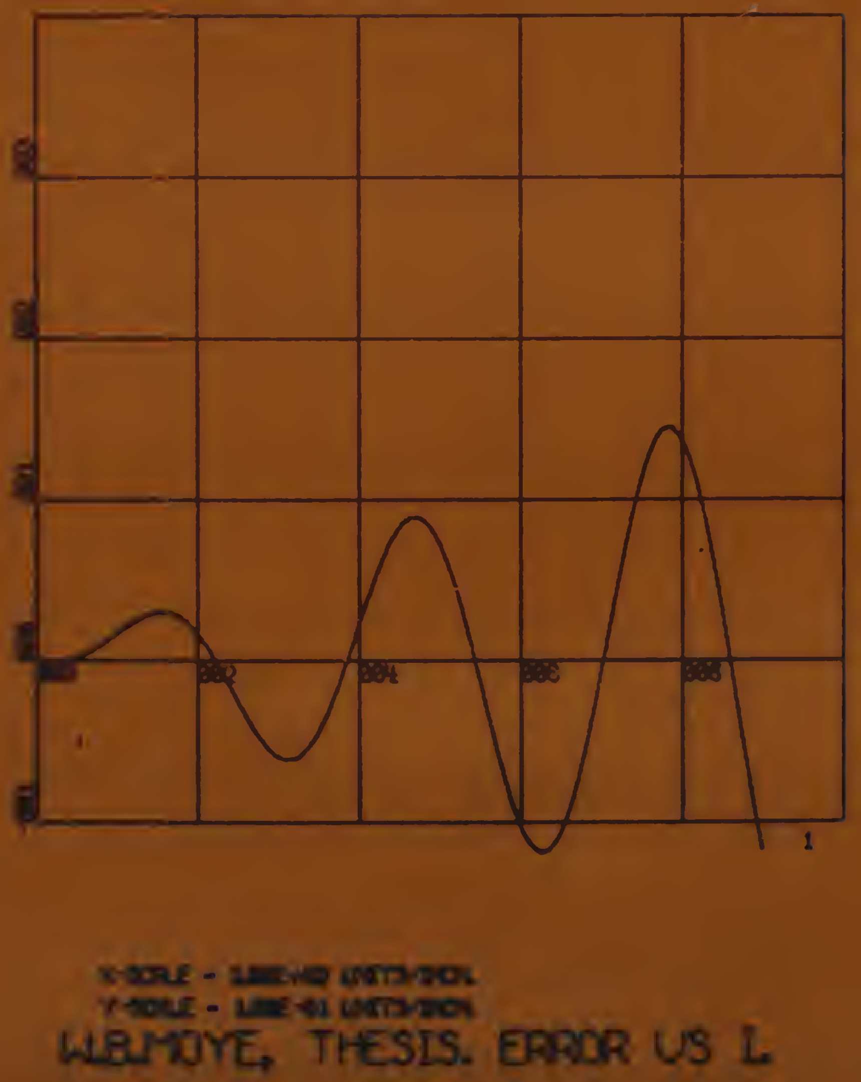


Fig. 8 - Formula 2 Error
Step length = .02

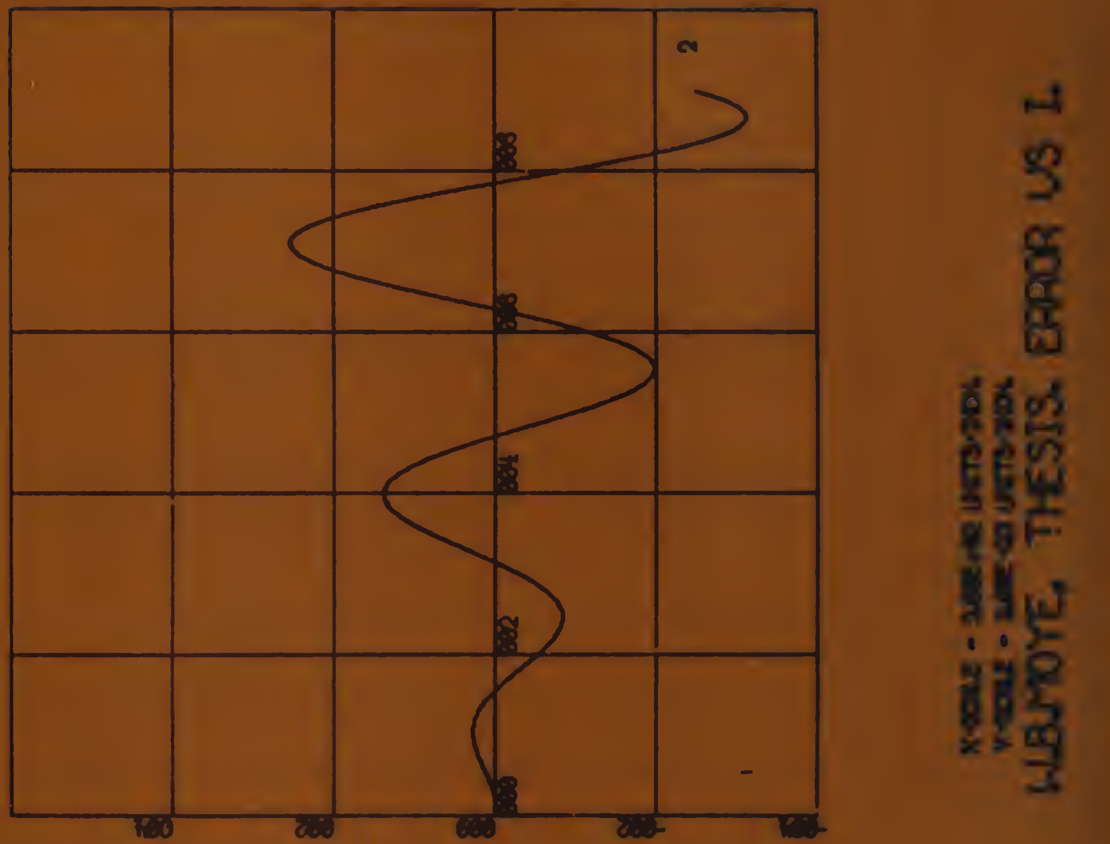


Fig. 9 - Formula 3 Error
Step length = .02

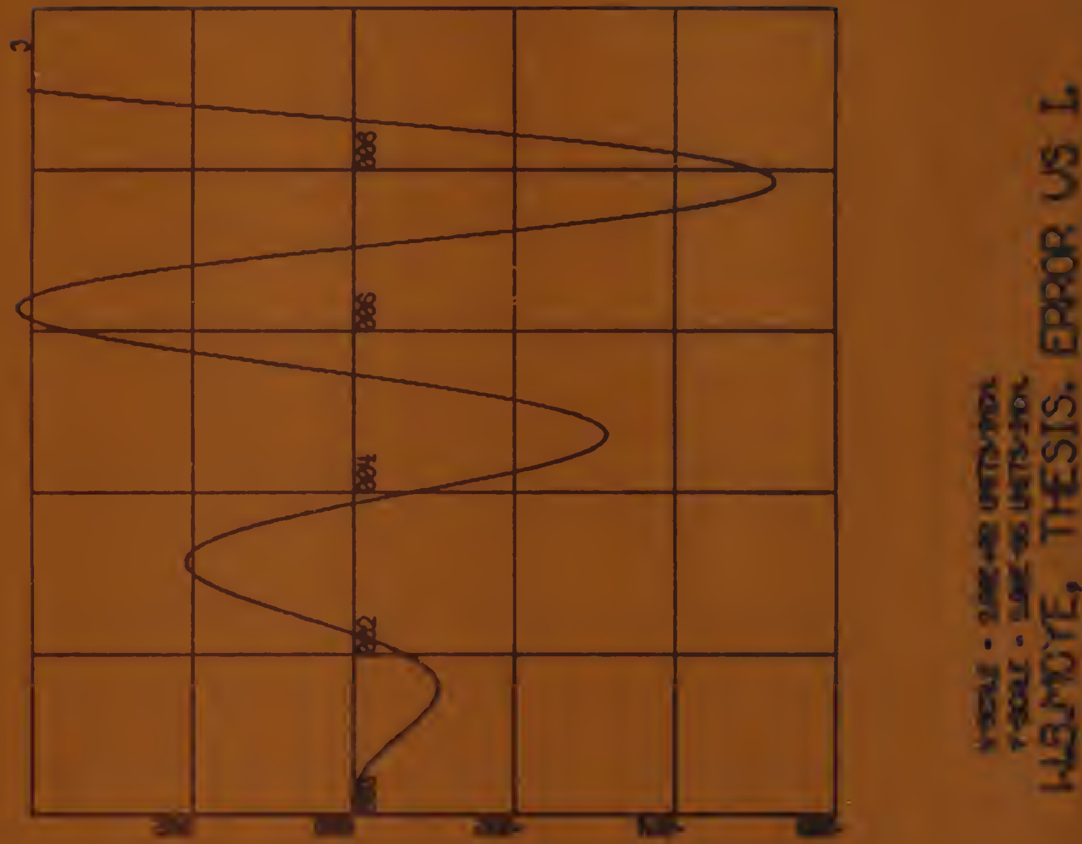


Fig. 10 - Formula 4 Error
Step length = .08

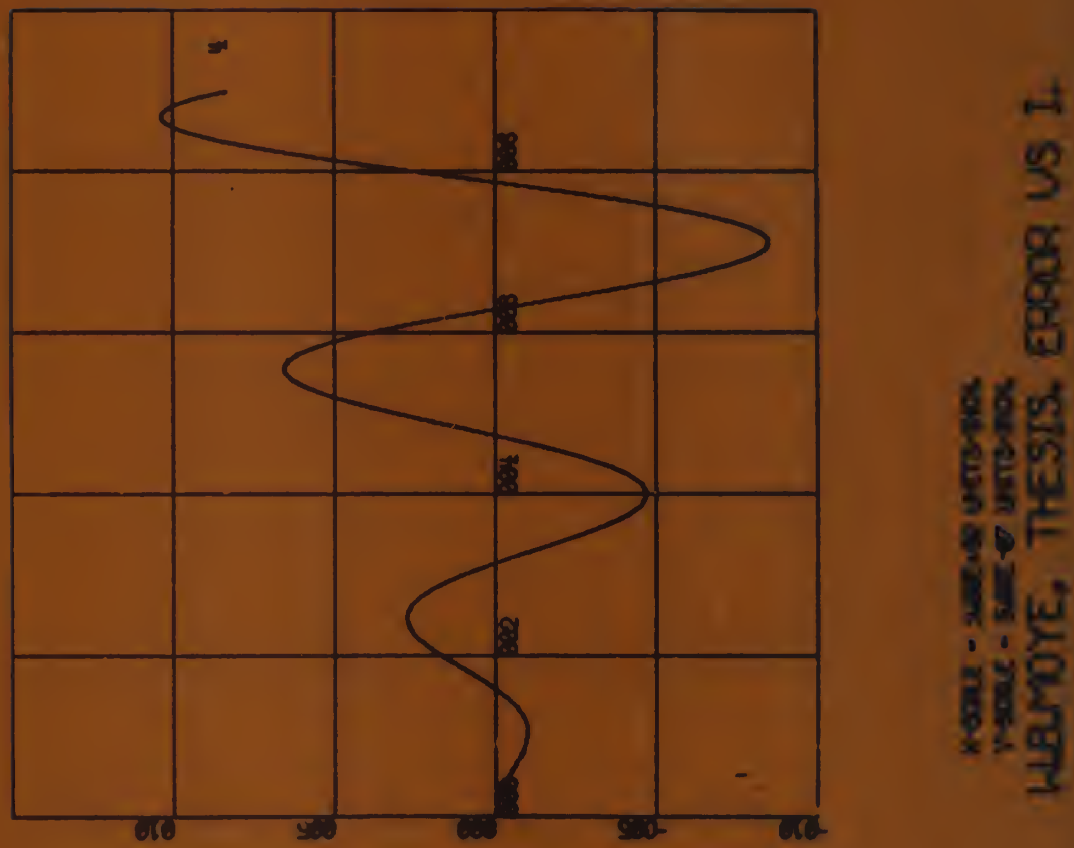
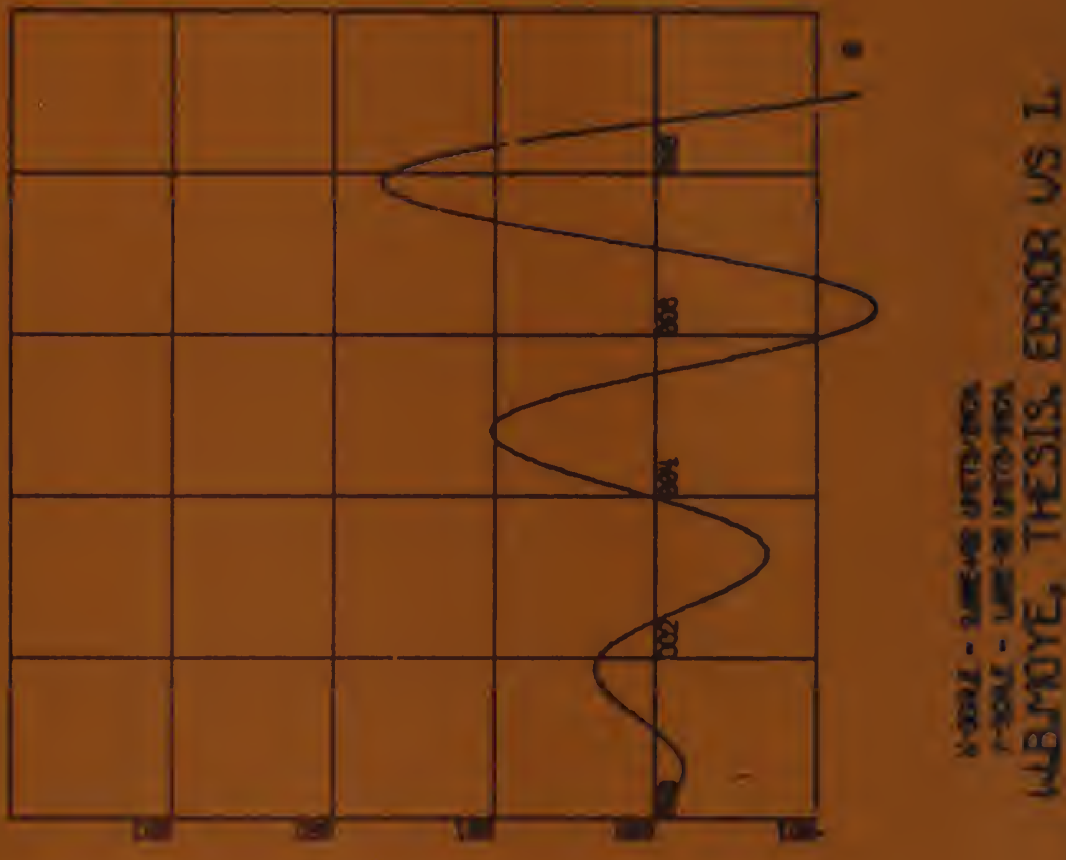


Fig. 11 - Formula 5 Error
Step length = .08



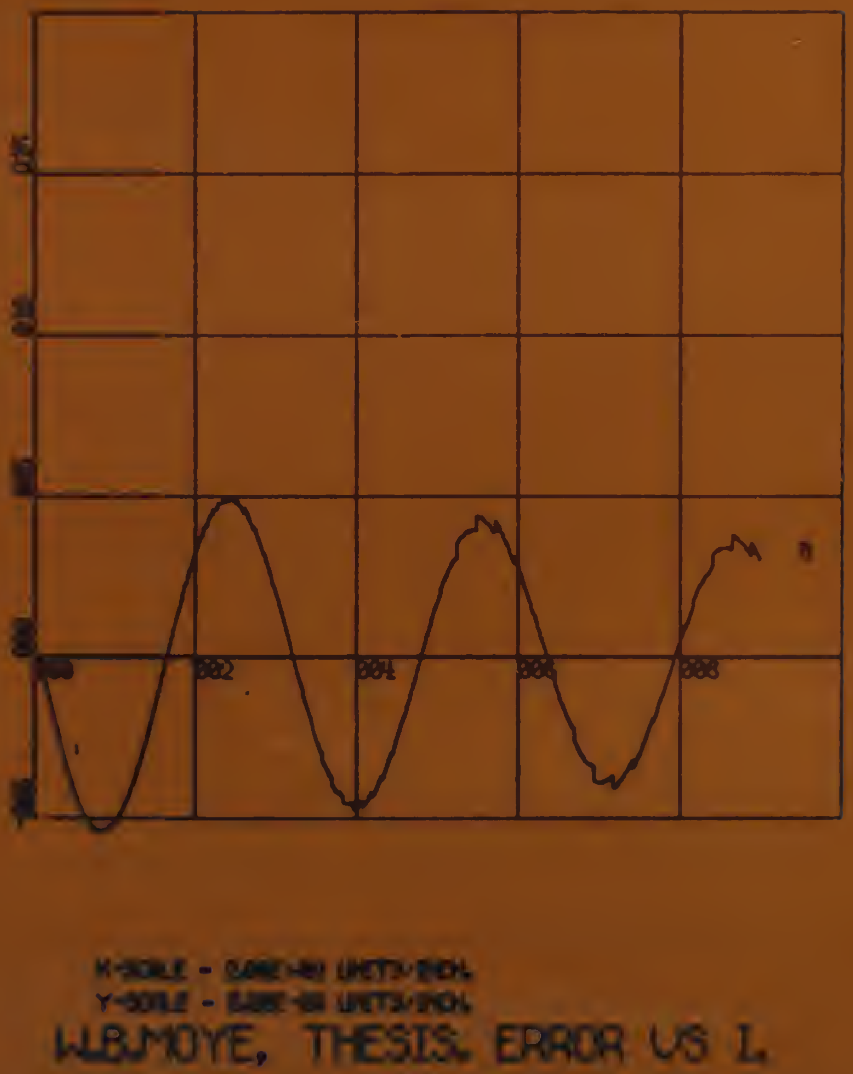


Fig. 18 - Formula 1 Error,
Step length = .06

Fig. 17 - Formula 7 Error
Step length = .02

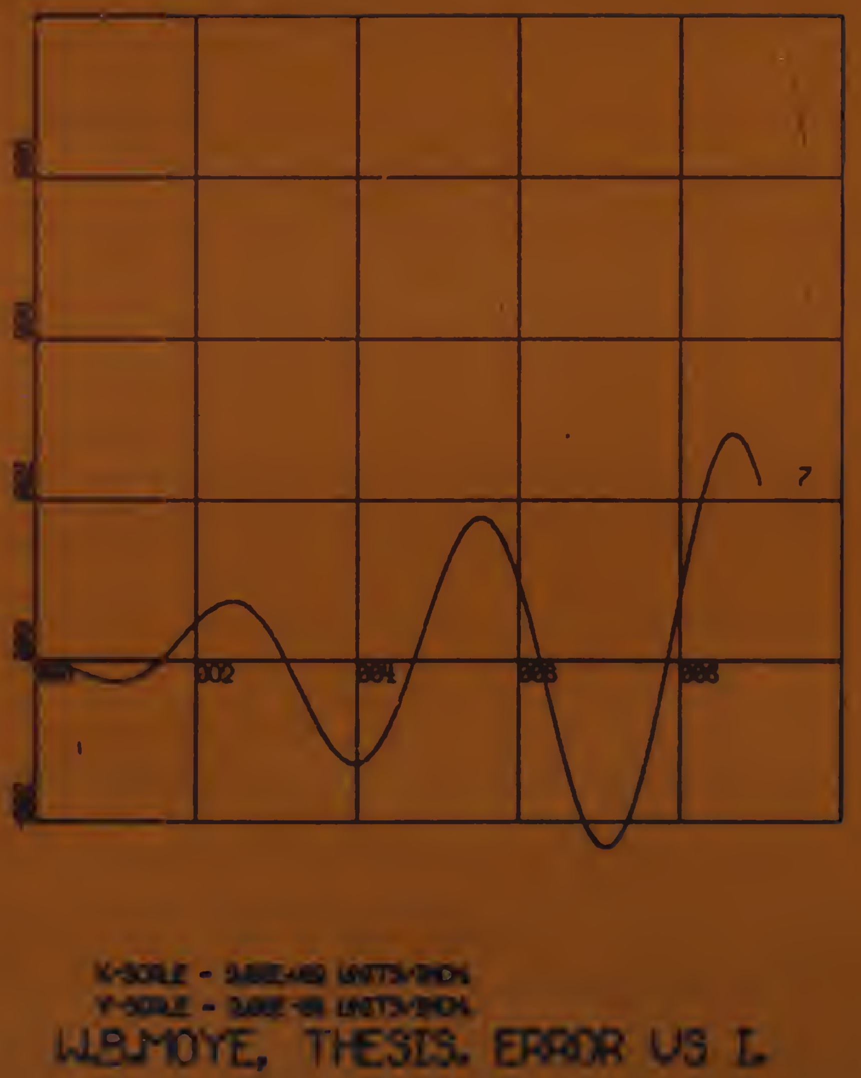
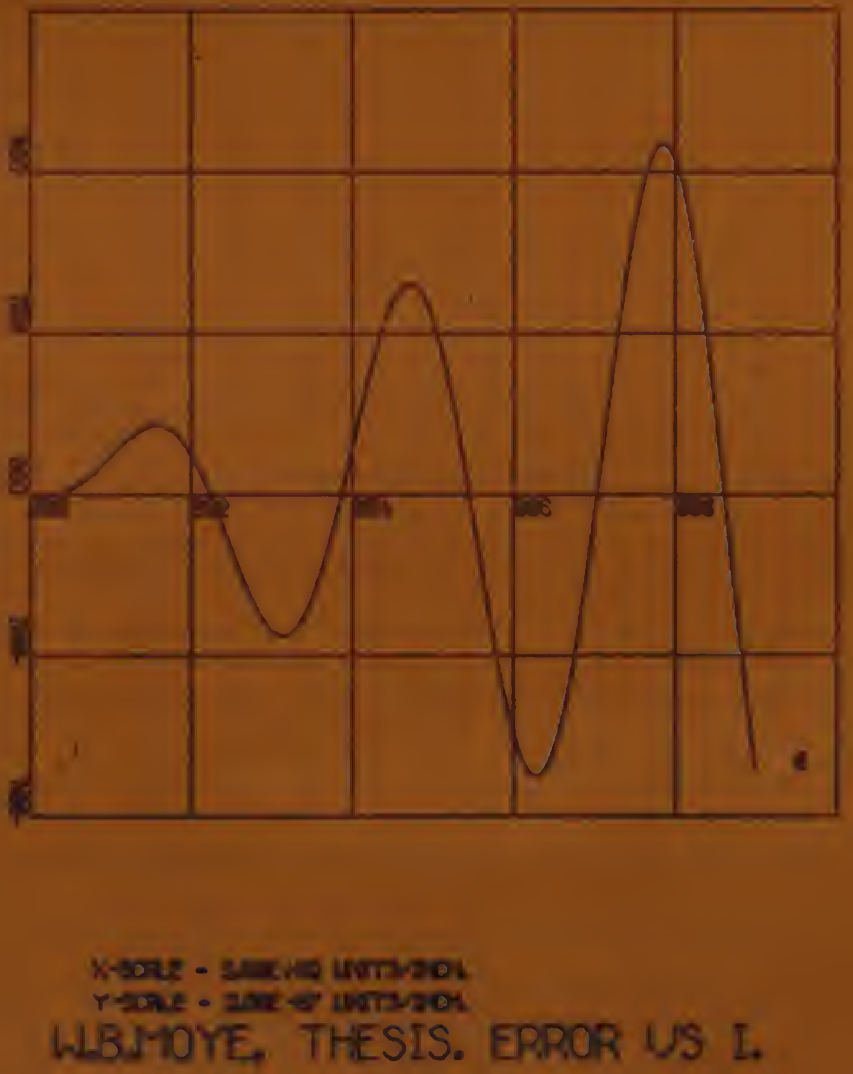


Fig. 14 - Formula F Error
Step length = .10



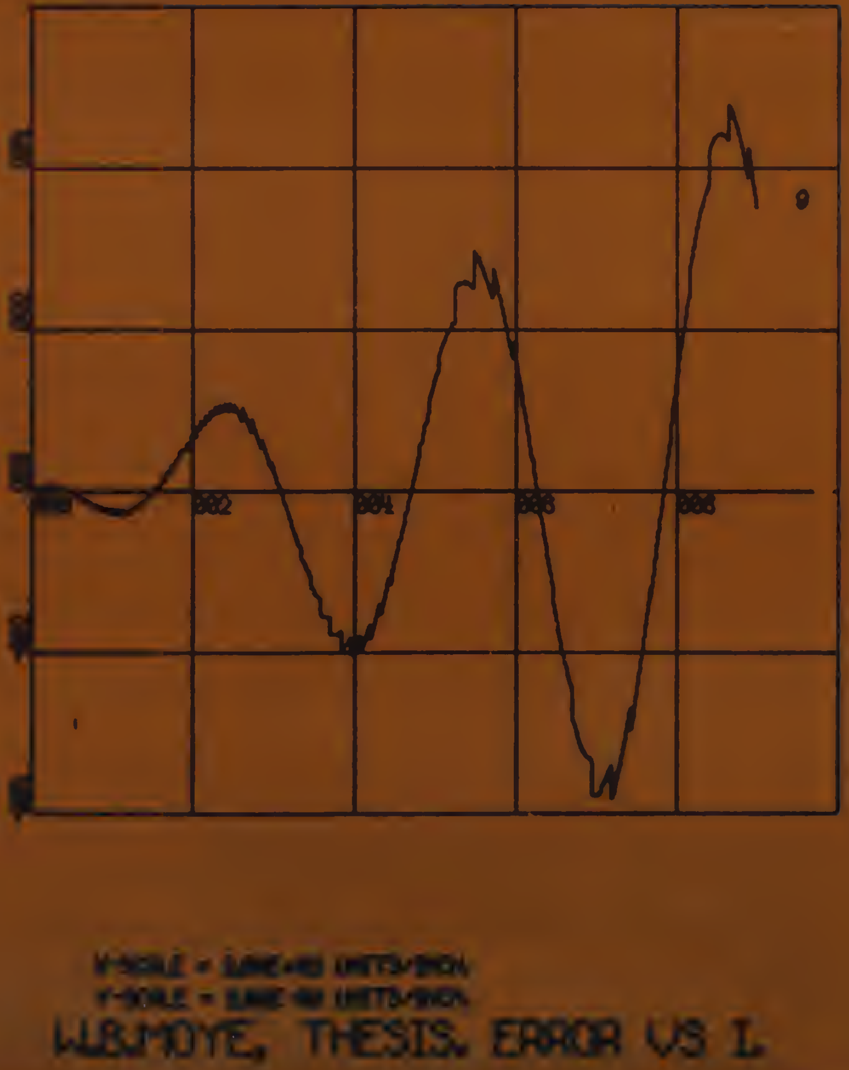
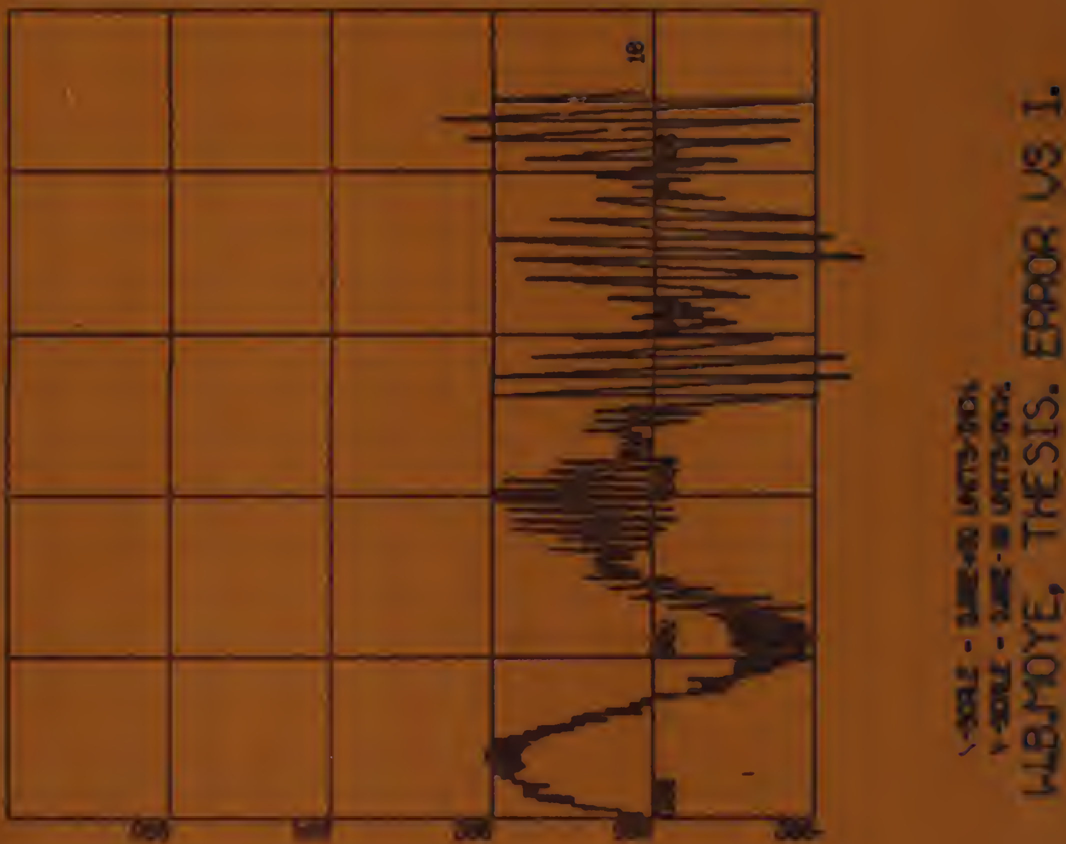


Fig. 15 - Formula 9 Error
Step length = .02

Fig. 16 - Formula 10 Error
Step length = .02



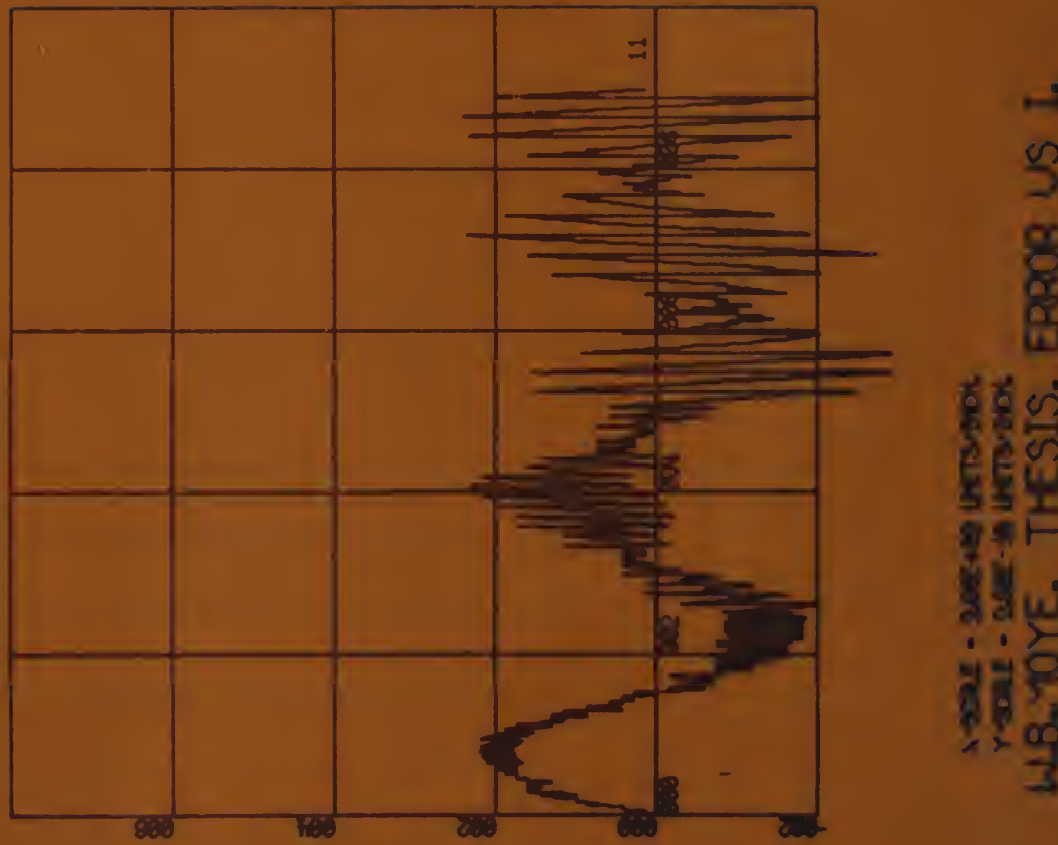


Fig. 17 - Formula 11 Error
Step Length = .02

Fig. 18 - Formula 12 Error
Step length = .02

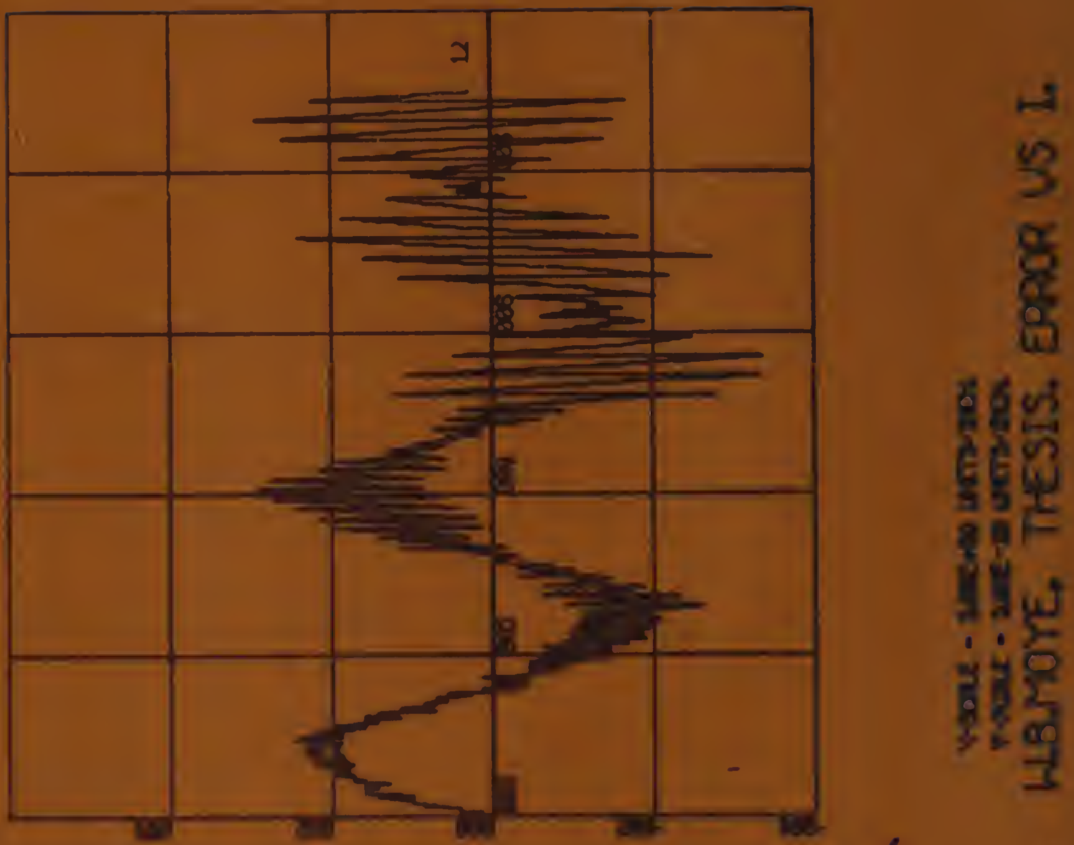


Fig. 19 - Formula 13 Error
Step length = .06

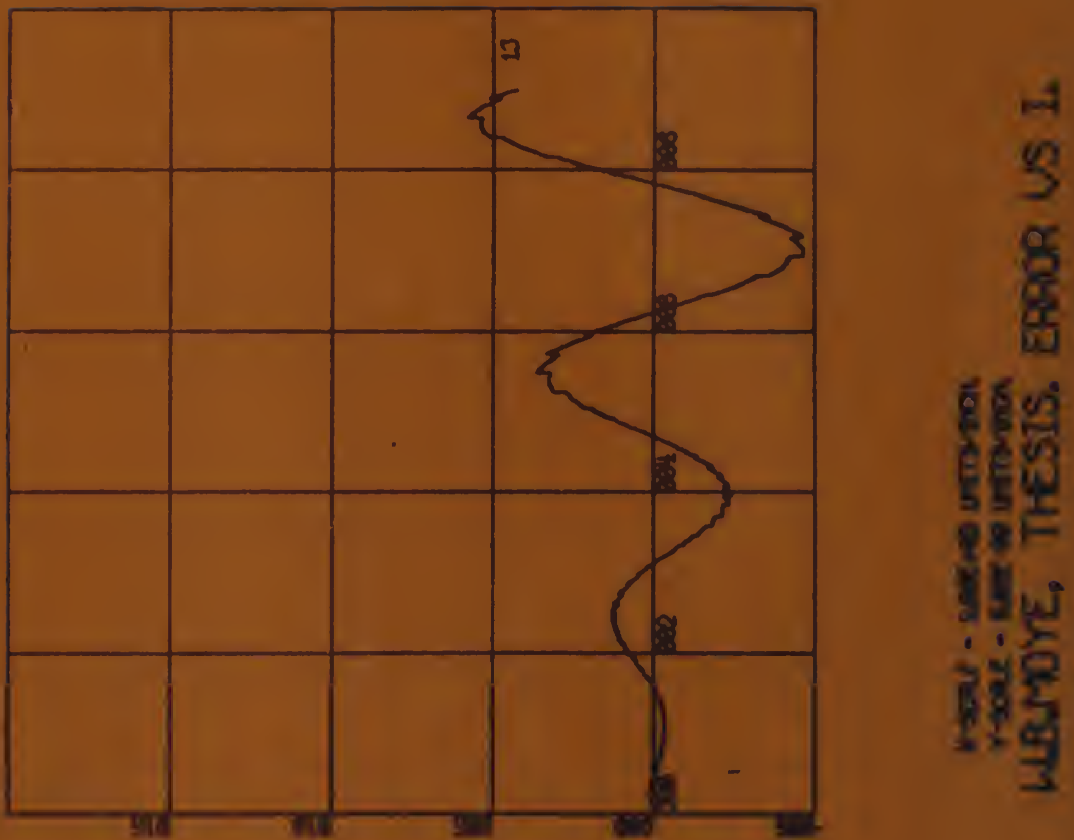
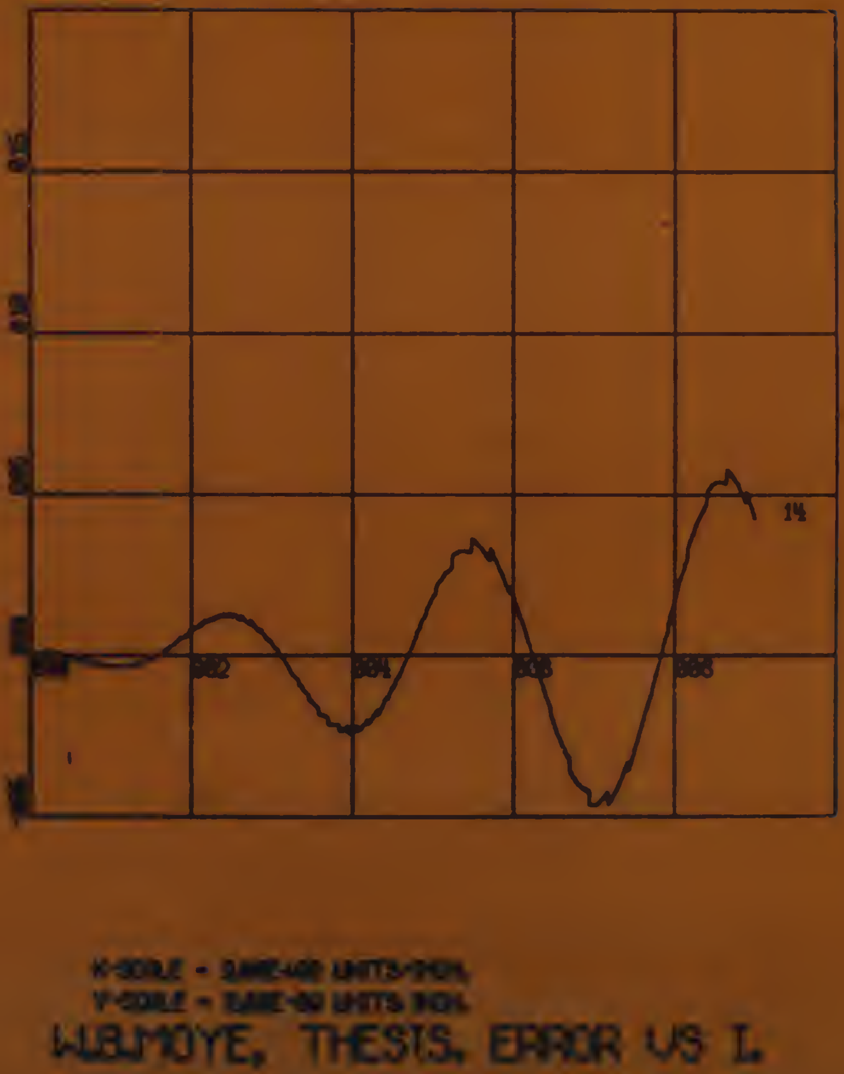


Fig. 30 - Formula 14 Error
Ray length = .06



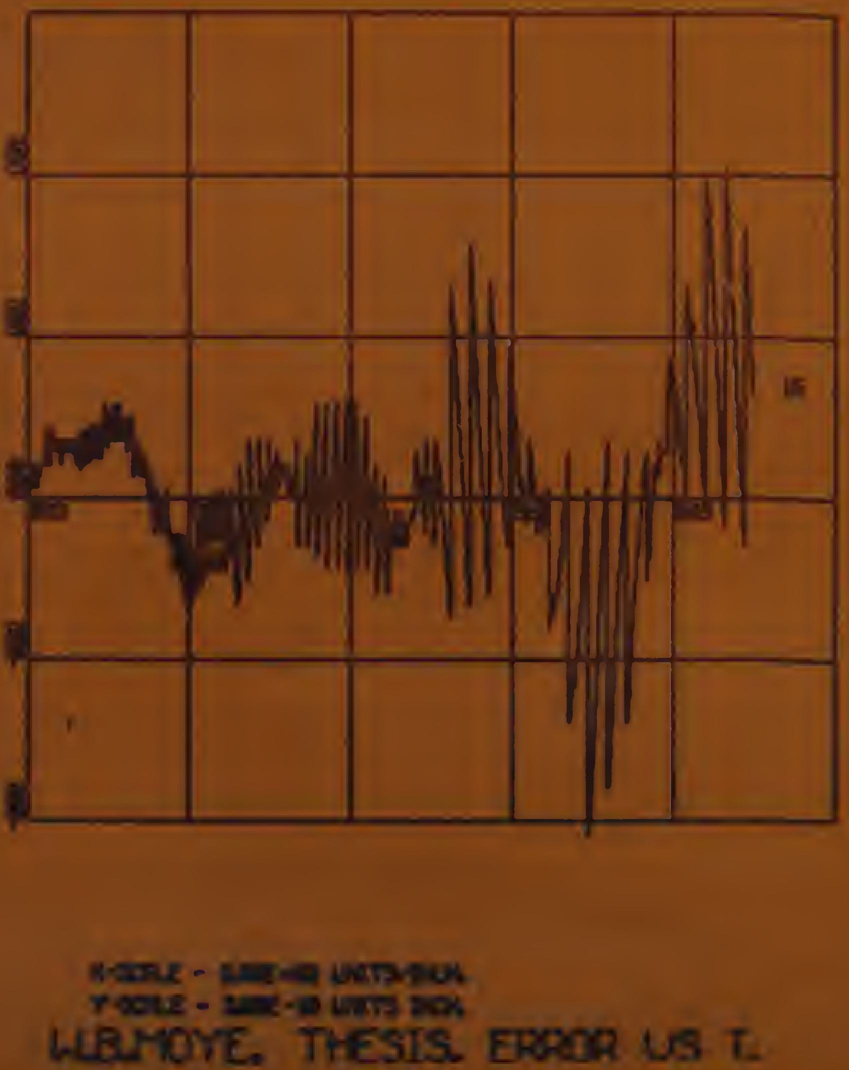


Fig. 21 - Formula 15 Error
Step length = .02

Fig. 27 - Formula 18 Error
Step length = .02

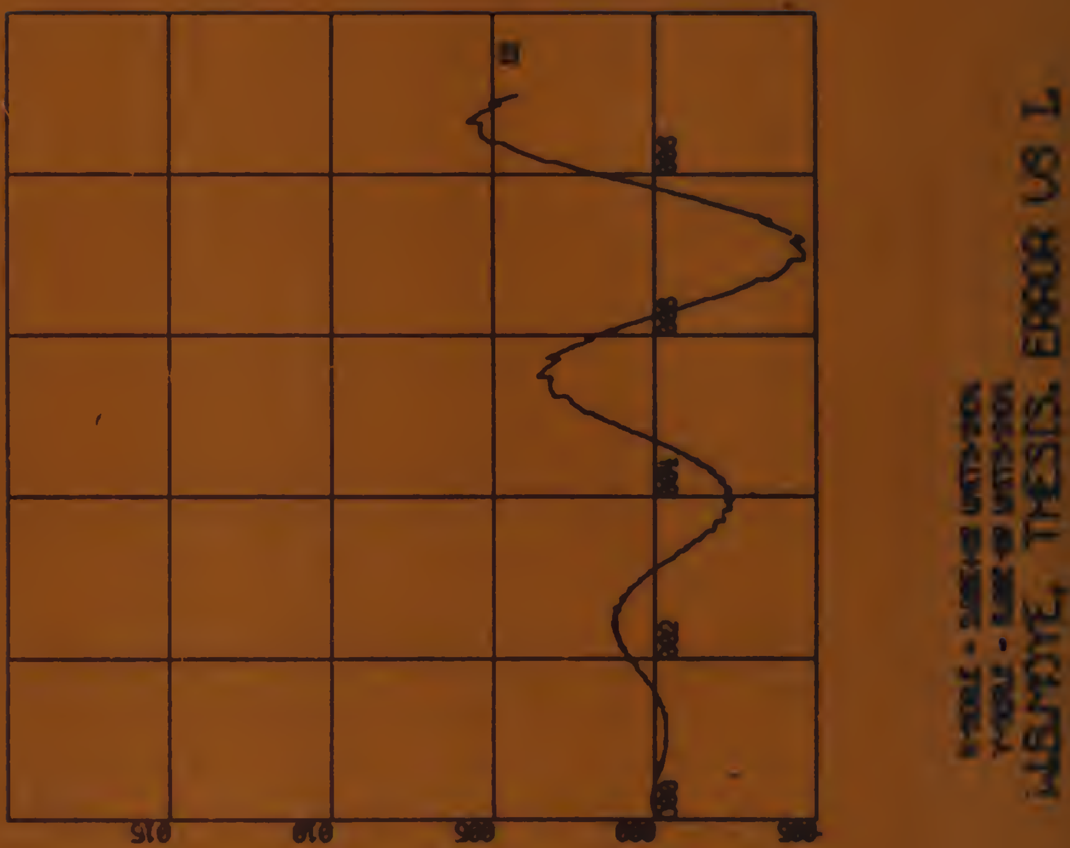


Fig. 13 - Formula 19 Error
Step length = .08

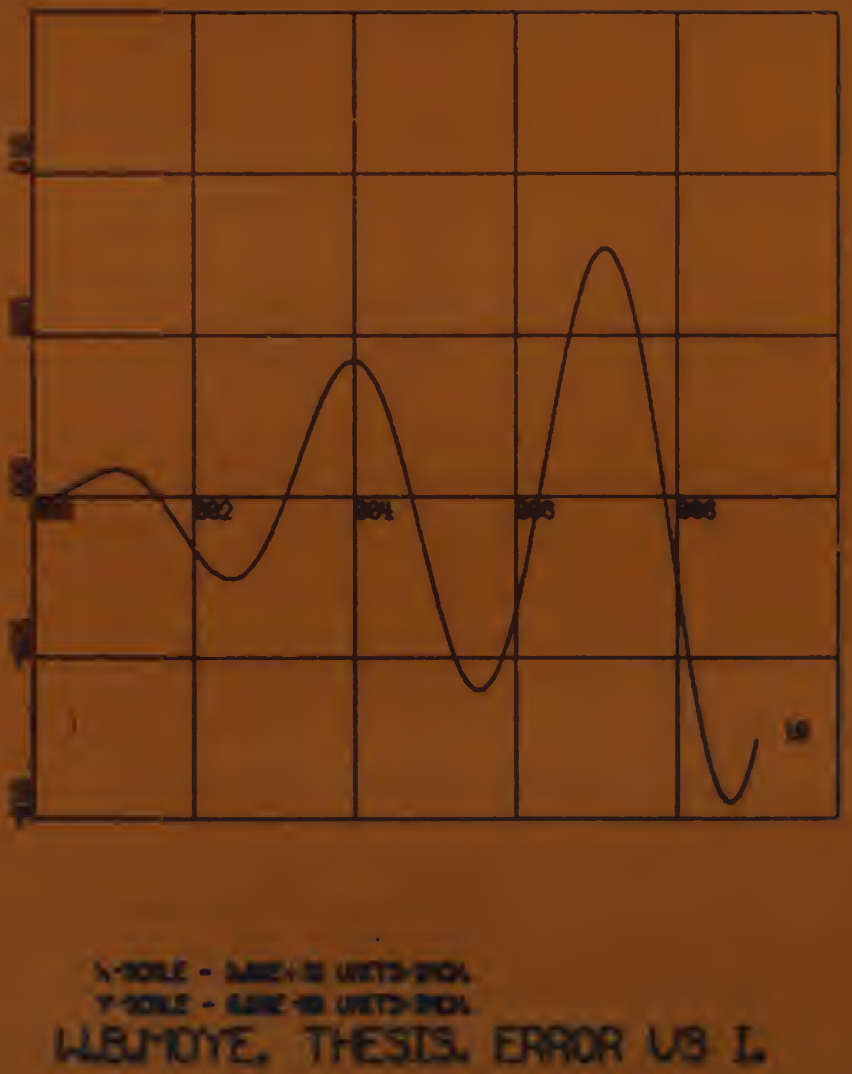


Fig. 39 - Formula 22 Error
Plug length = .08

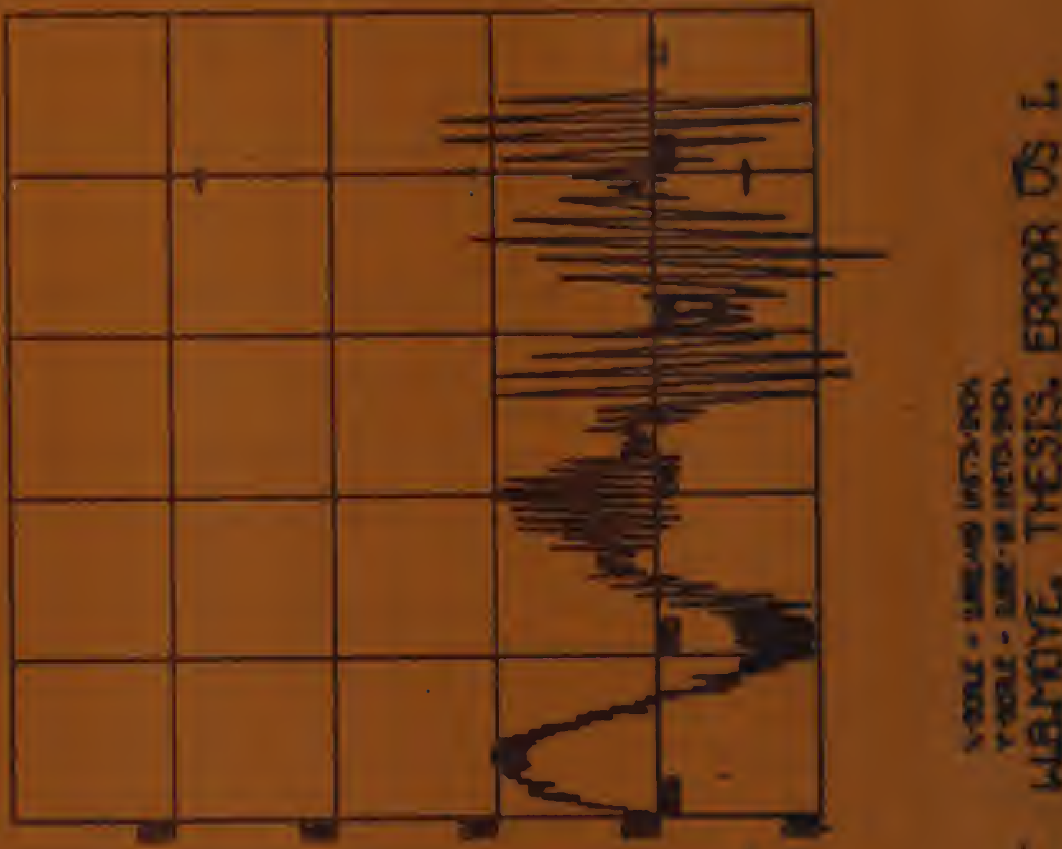


Fig. 31 - Formula 25 Error
Step Length = .08

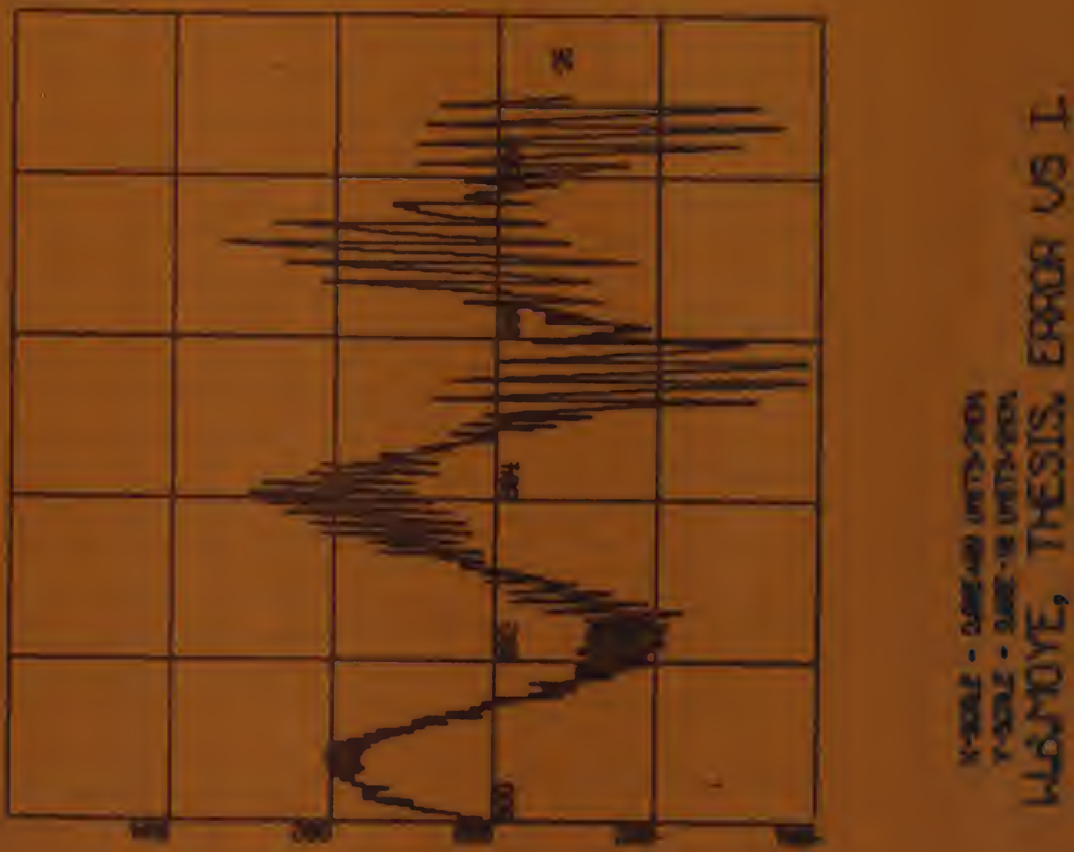


Fig. 18 - Formula 3 Error
Step Length = .01

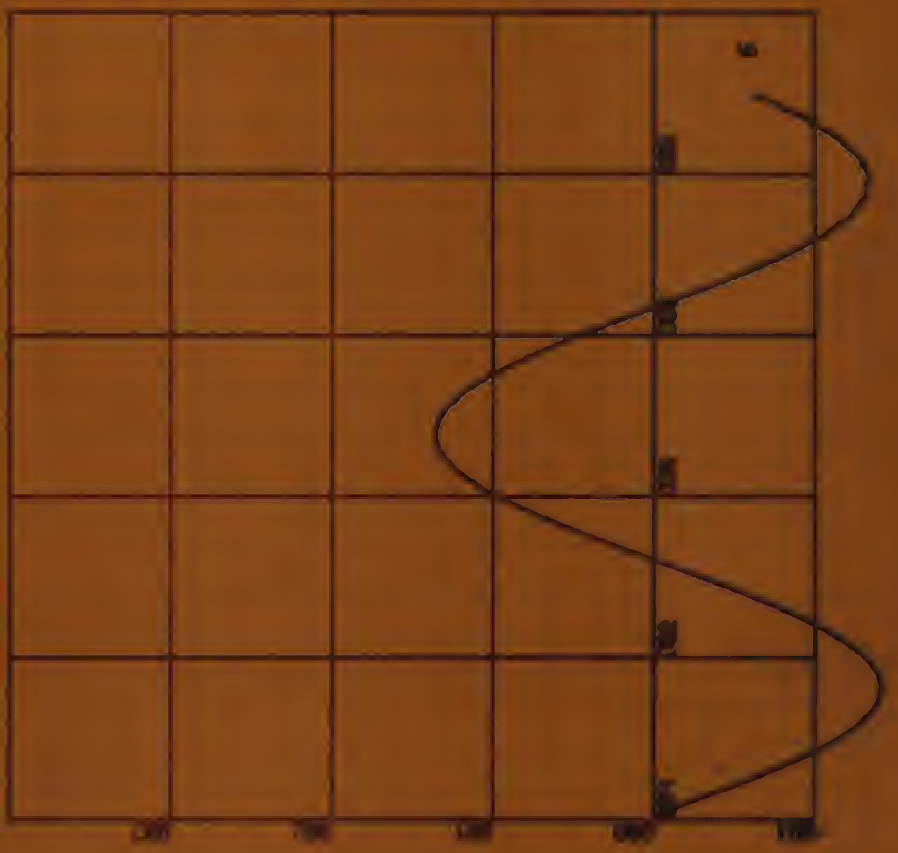


Fig. [illegible] - Formula 6 Error
Step length = .01

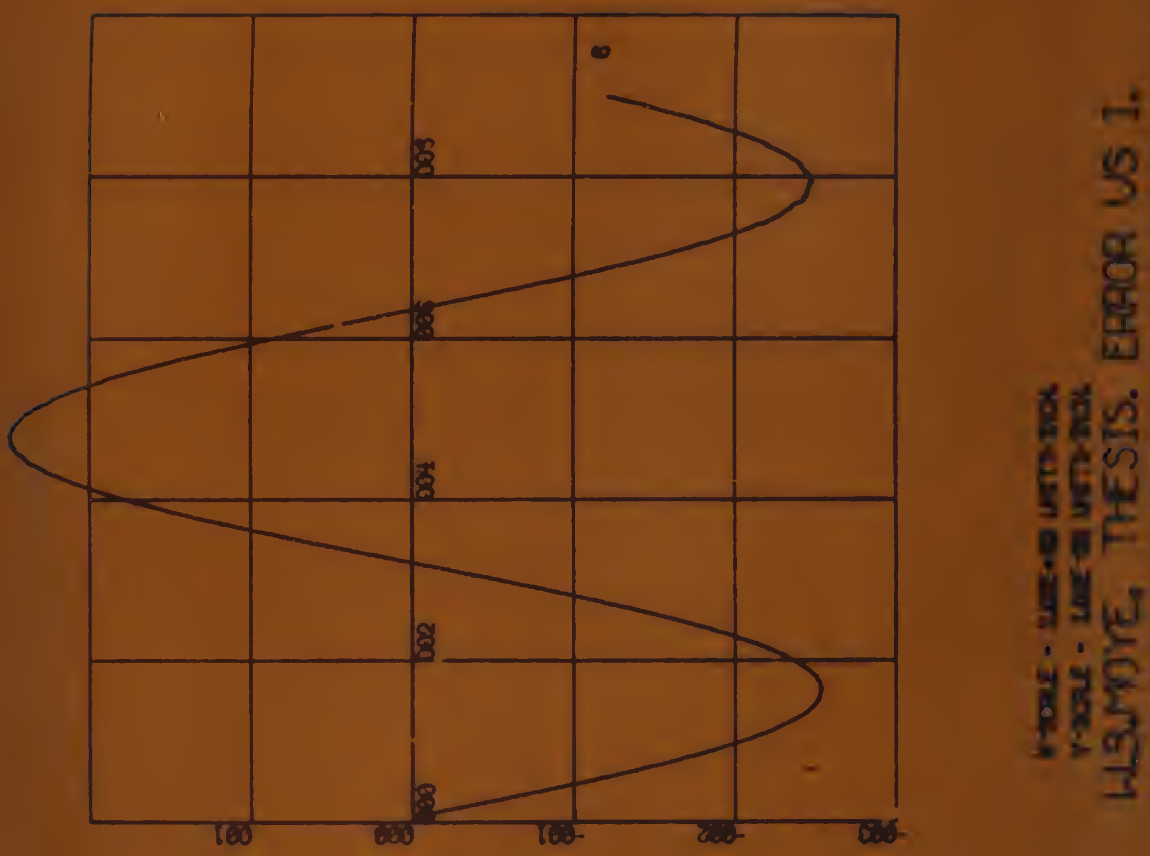


Fig. 17 : Formula 10 Error
Step Length = .01

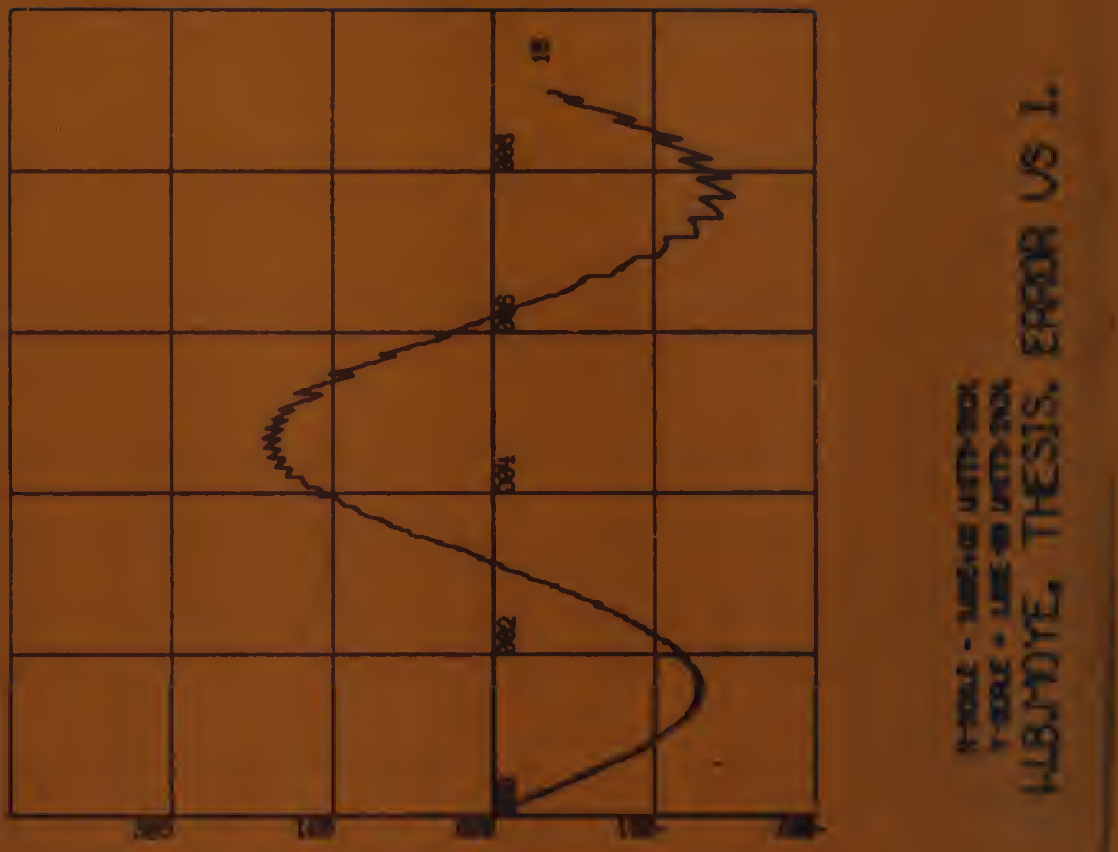


Fig. [illegible] . Formula [illegible] Error
Wave Length = [illegible]

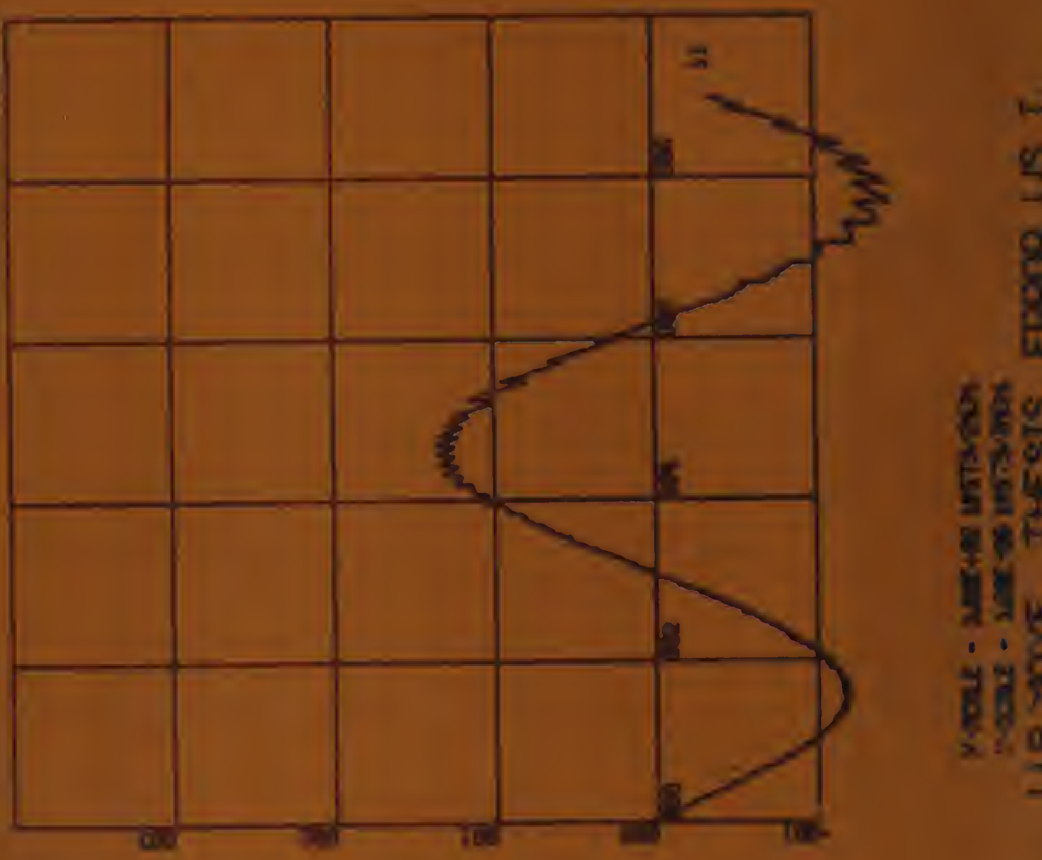


Fig. 37 - Formula 17 Error
Step length = .01

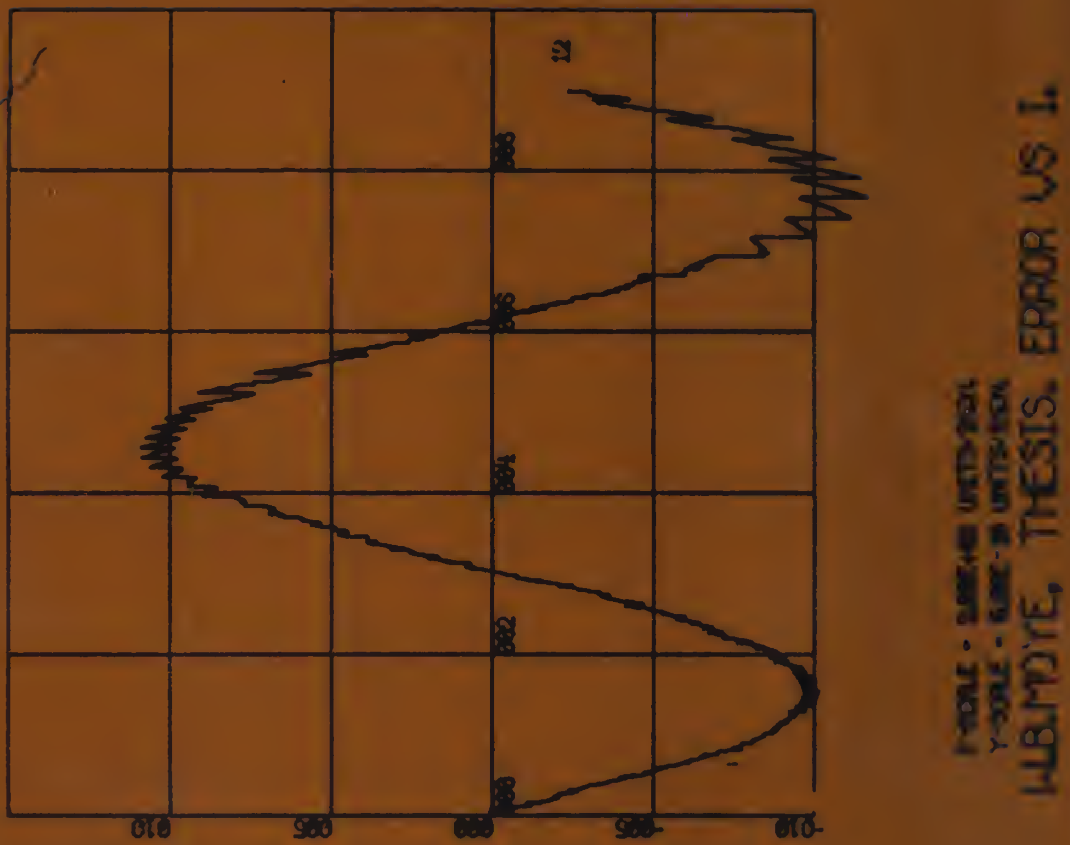


Fig. 31 - Formula 11 Error
Step length = .01

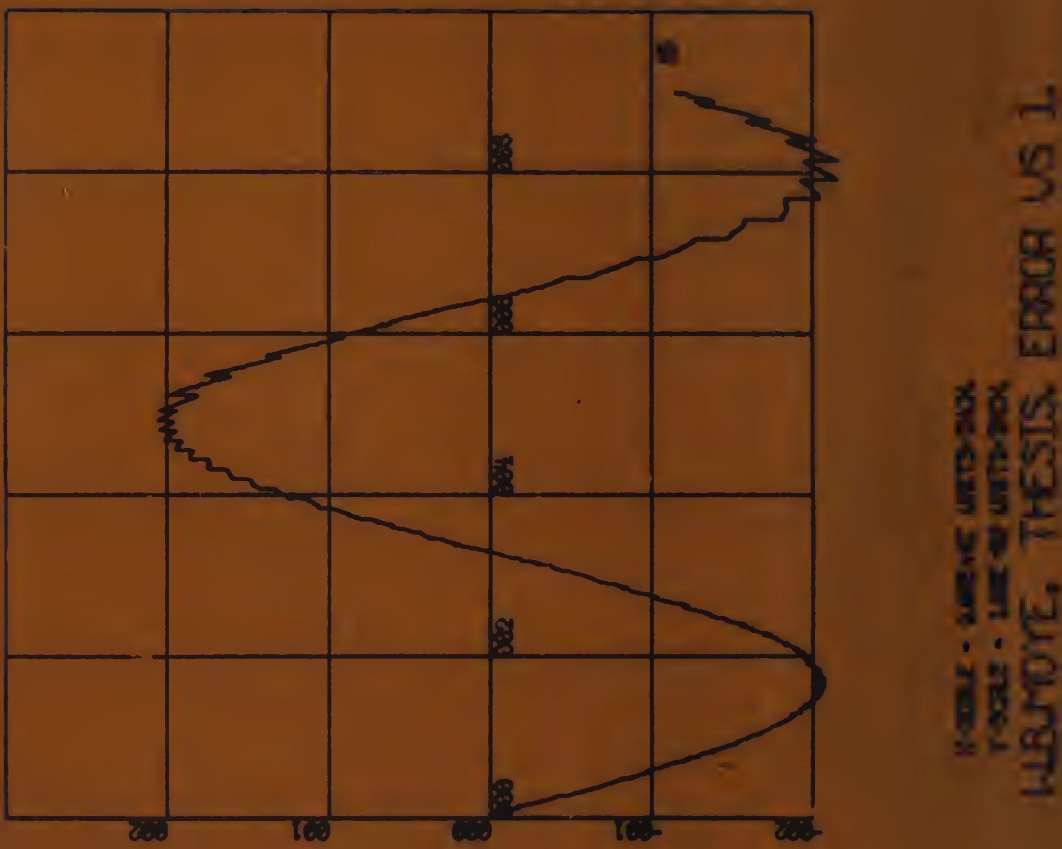


Fig. 32 - Formula 22 Error
Step length = .31

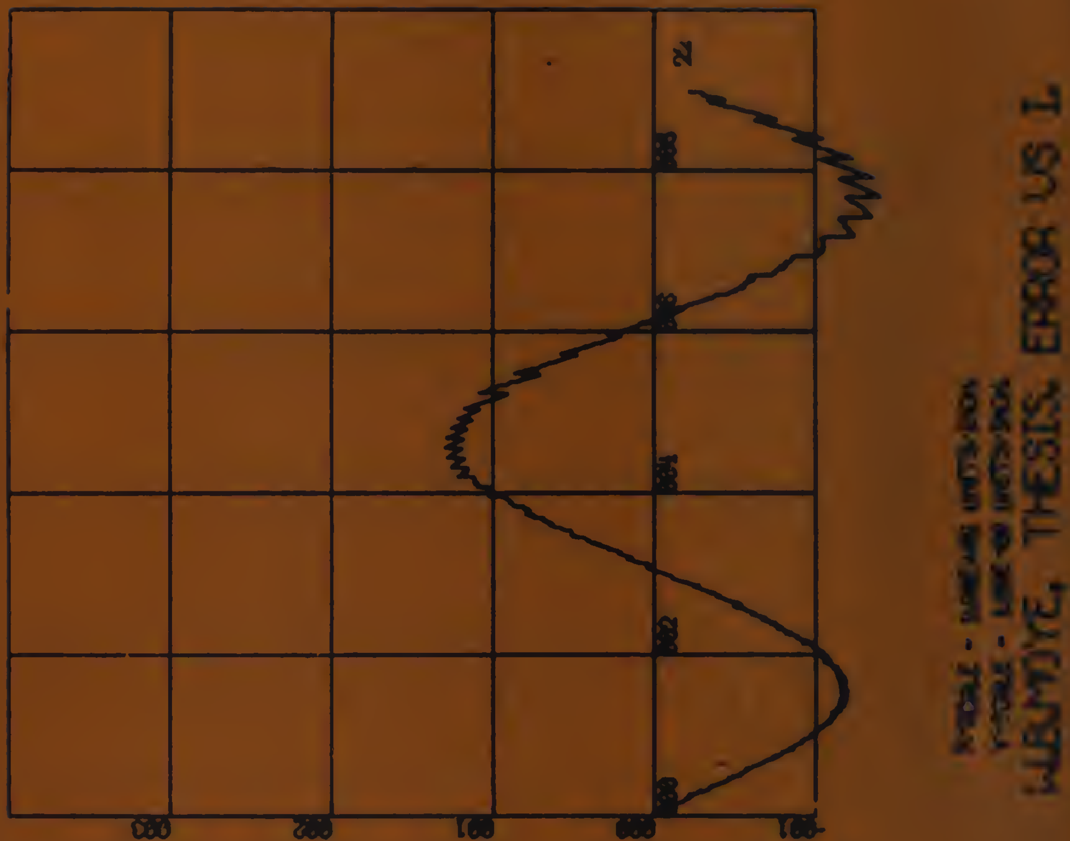


Fig. 11 - Formula 13 Error and Formula 12 Error
Step Length = .01 Step Length = .03

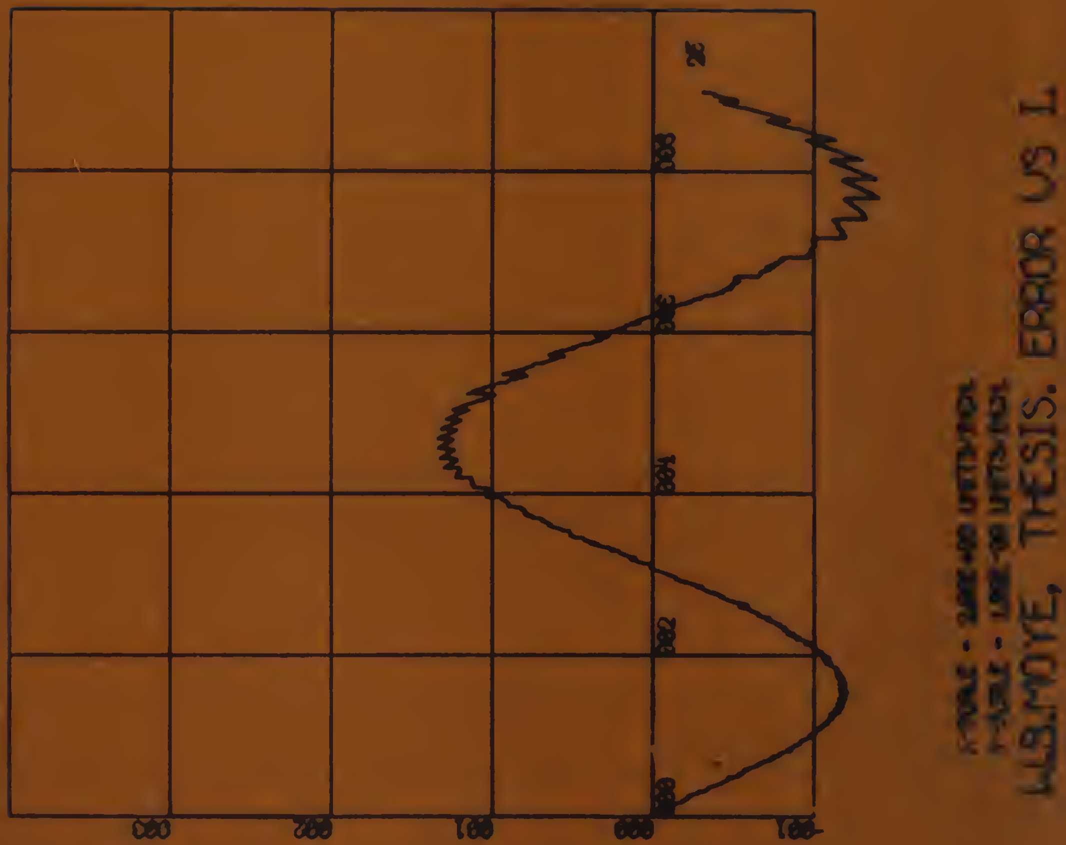
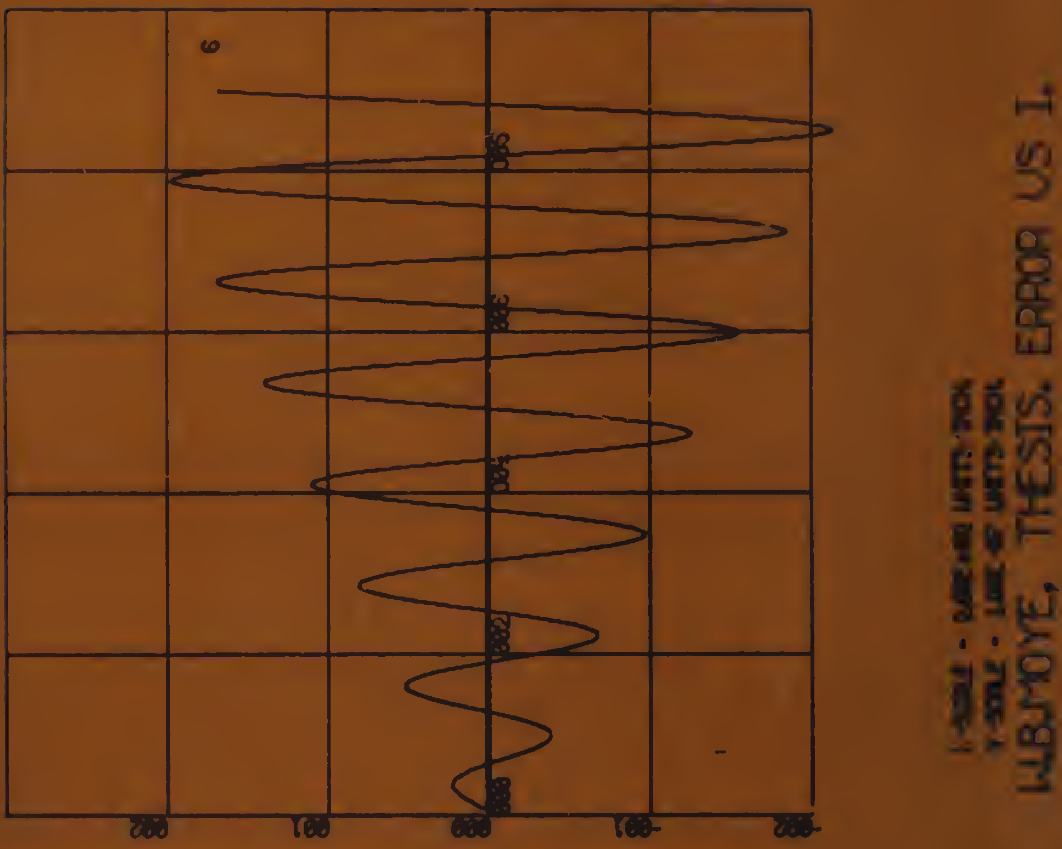


Fig. [illegible] - Formula 6 Error
Step Length = .08



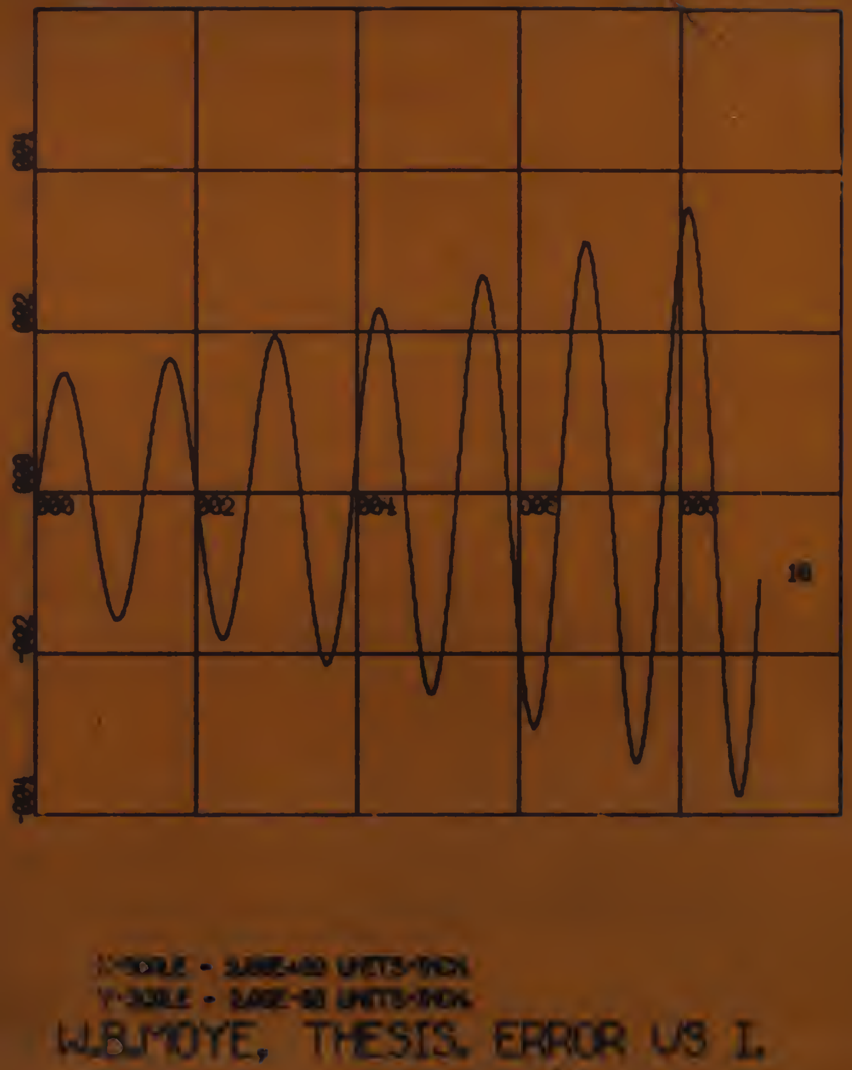
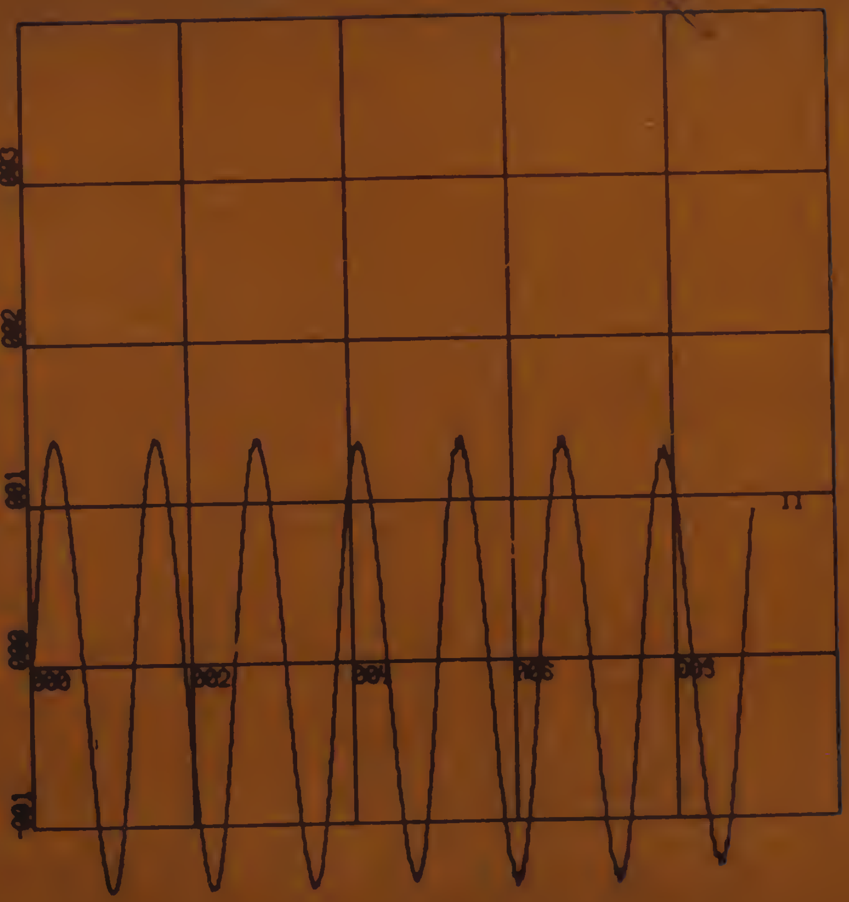


Fig. 33 - Formula 10 Error
Step length = .05

Fig. 35 - Formula 11 Error
Step length = .05



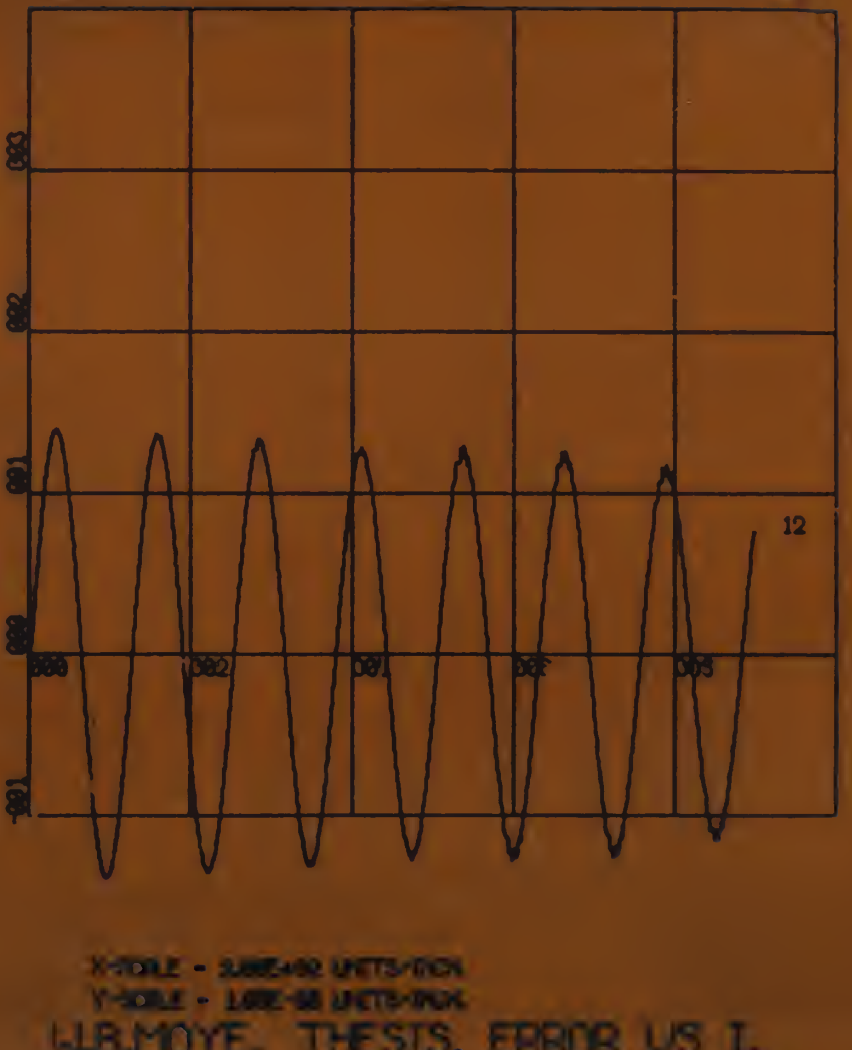


Fig. [illegible] - Formula 12 Error
Step Length = .05

Fig. 38 - Formula 15 Error
Step length = .05

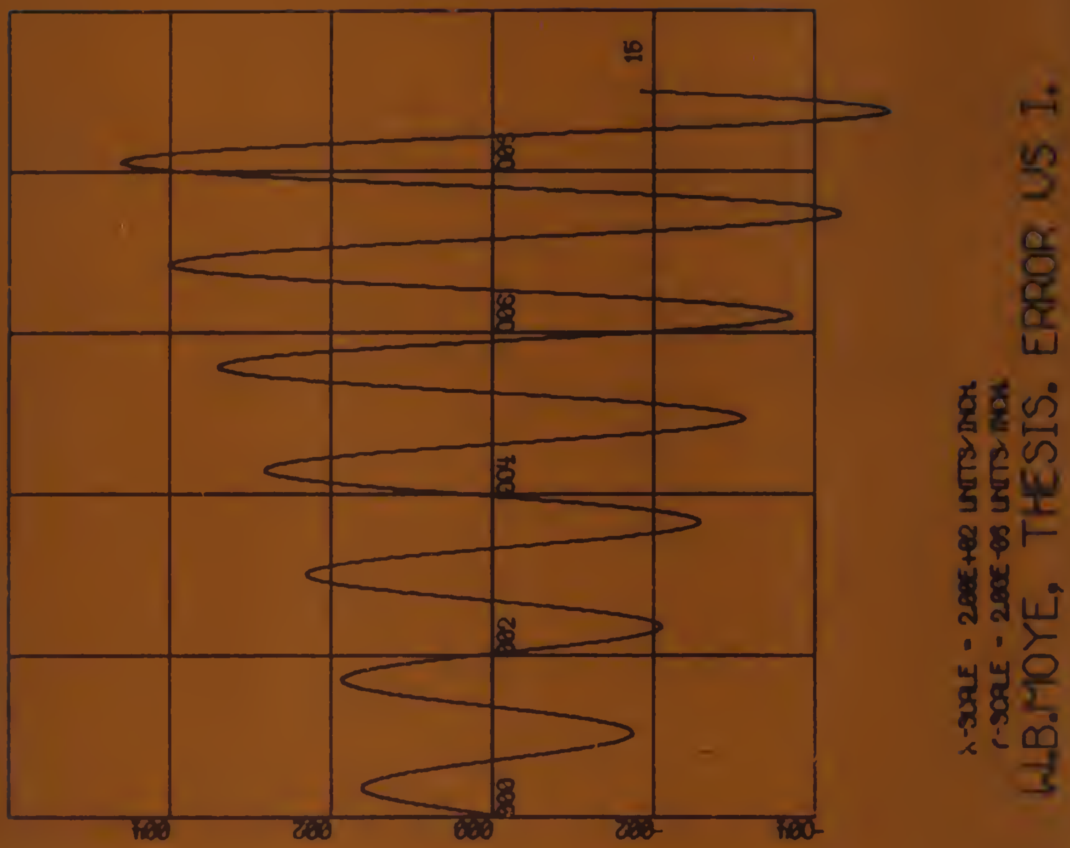


Fig. [illegible] - Formula 32 Error
For Sample = .05

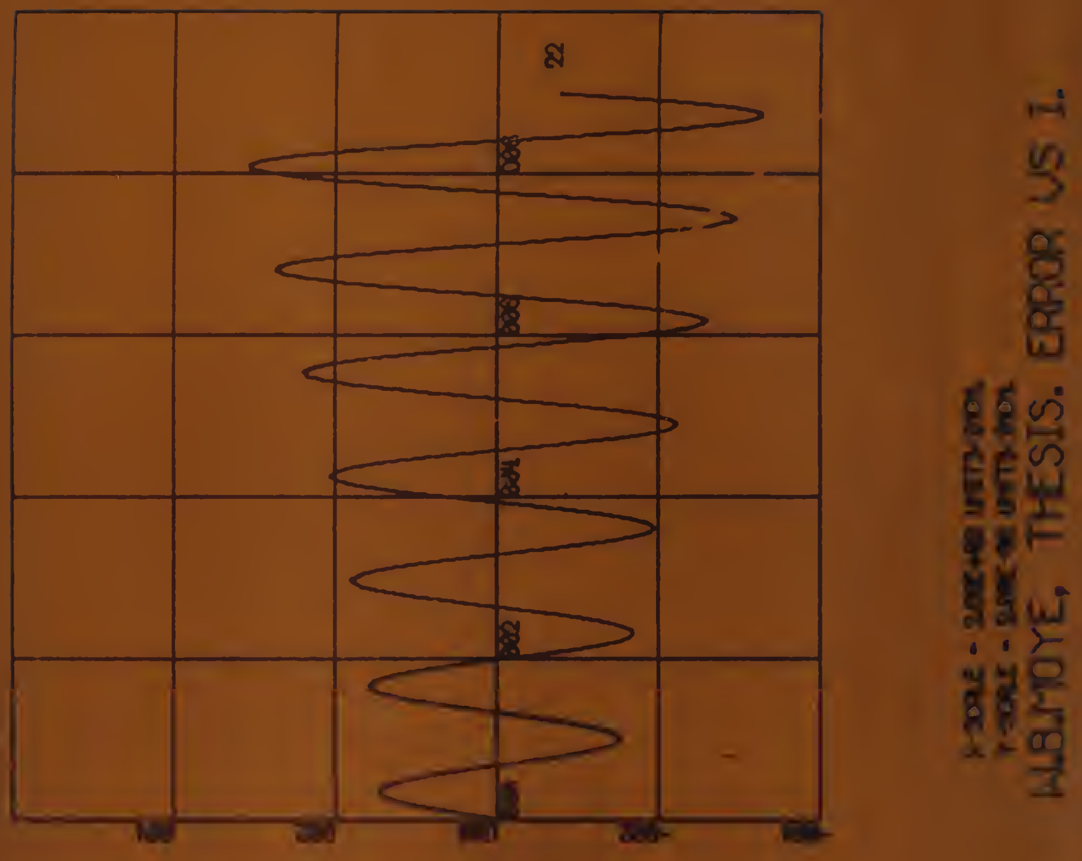


Fig. [illegible] - Formula 83 Error
Step length = .05

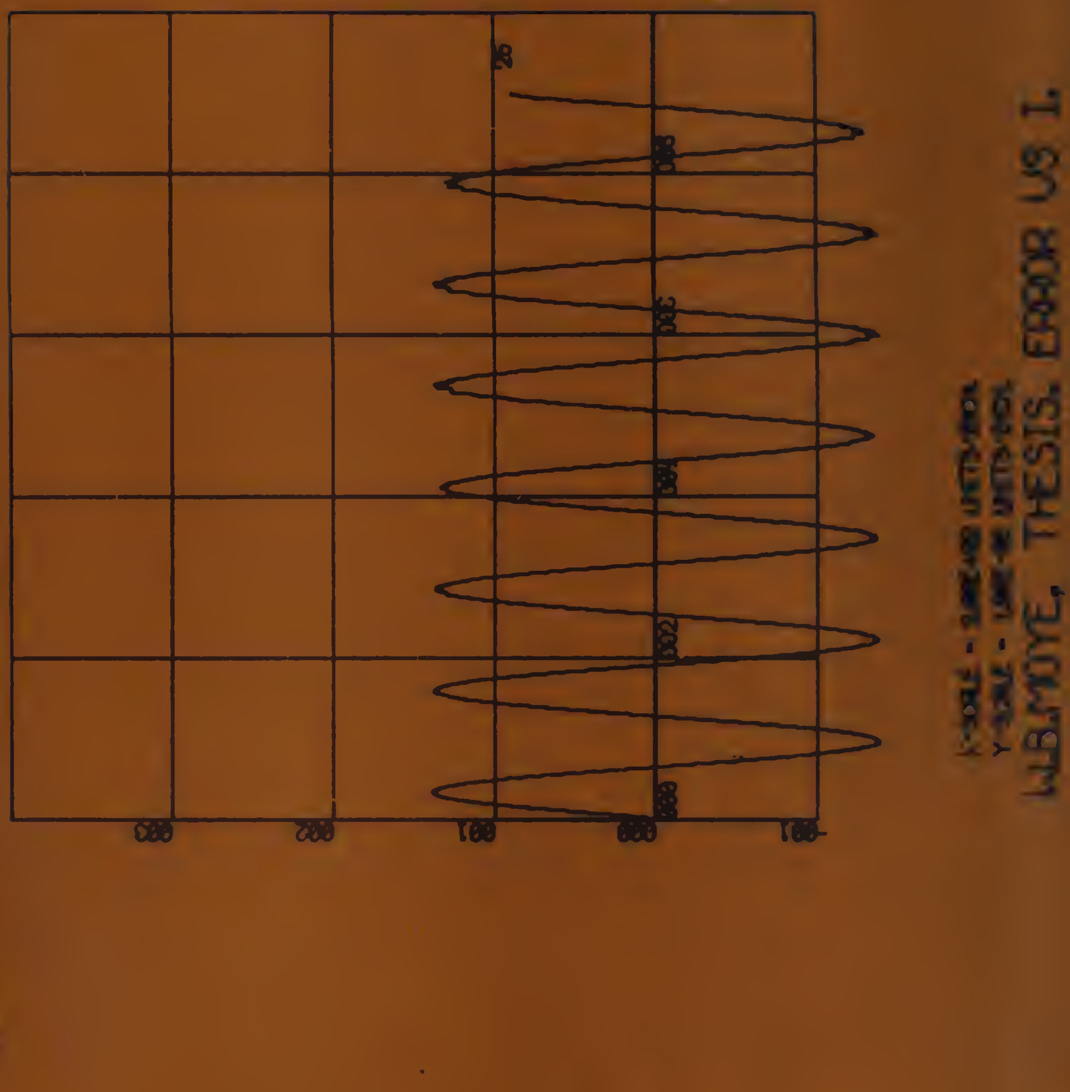


Fig. [illegible] - Formula [illegible] Error
Step Length = .05

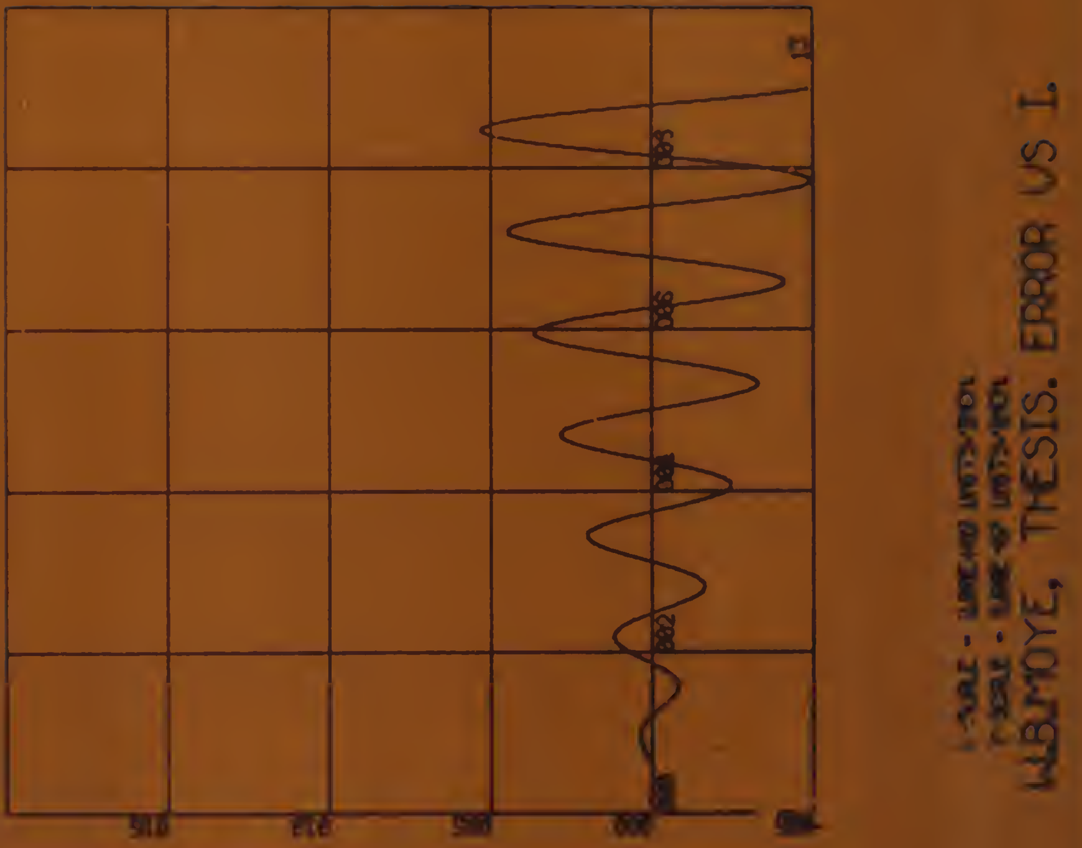


Fig. 42 - Solution error; Coulomb Wave Equations

Equations	$y''+y(1-2/x-2/x^2)=0$				$y''+y(1-6/x-[illegible])=0$			
Step	.01	.02	.05	.1	.01	.02	.05	.1
Formula No.								
1	9E-3	2E-1	4E-2	8E-1	5E-1	----	----	----
2	5E-5	2E-3	1E-2	3E-3	4E-3	2E-2	5E-2	1E-1
3	4E-7	3E-5	5E-5	5E-4	9E-6	6E-5	3E-4	[illegible]
4	----	----	----	----	----	----	----	----
5	----	----	----	----	----	----	----	----
6	----	----	----	----	----	----	----	----
7	5E-7	2E-4	9E-5	2E-4	3E-4	1E-3	5E-3	1E-2
8	0	0	4E-7	4E-6	0	0	3E-5	5E-4
9	0	0	0	1E-7	0	1E-7	3E-5	5E-4
10	7E-4	5E-3	4E-4	4E-4	2E-1	2E-1	9E-2	1E-1
11	3E-3	2E-2	6E-6	1E-3	8E-1	8E-1	7E-1	6E-1
12	----	----	----	----	----	----	----	----
13	0	0	0	1E-7	0	1E-7	3E-5	5E-4
14	0	0	0	1E-7	0	1E-7	3E-5	5E-4
15	0	0	0	1E-7	0	1E-7	3E-5	5E-4
18	0	0	0	1E-7	0	1E-7	3E-5	5E-4
19	7E-4	5E-3	7E-5	5E-4	3E-1	2E-1	2E-1	2E-1
22	3E-2	3E-3	4E-4	1E-3	2E-1	2E-1	2E-1	2E-1
25	2E-3	1E-2	5E-4	3E-3	7E-1	7E-1	6E-5	5E-1
Iterations	400	200	80	40	400	200	80	40

Tabulated values are final solution error after number of iterations indicated. Dashes indicate error in excess of 1E+0 (1×10^0).

Fig. 5C - Milne Optimal Error
Step Length = .01

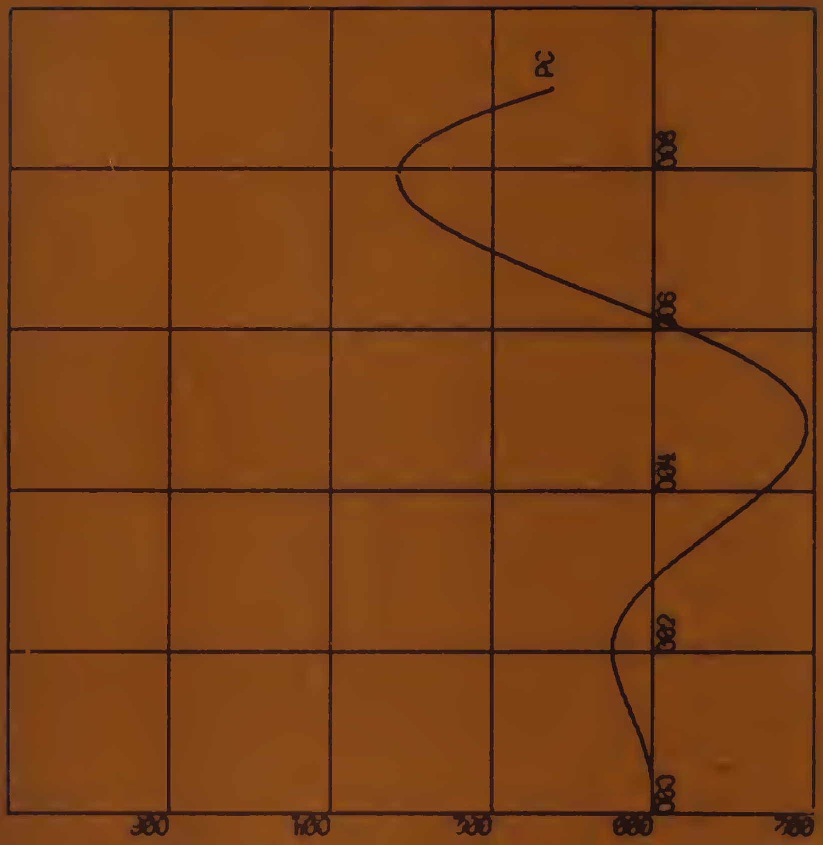


Fig. [illegible] - [illegible] Output Wave
[illegible] Length = [illegible]

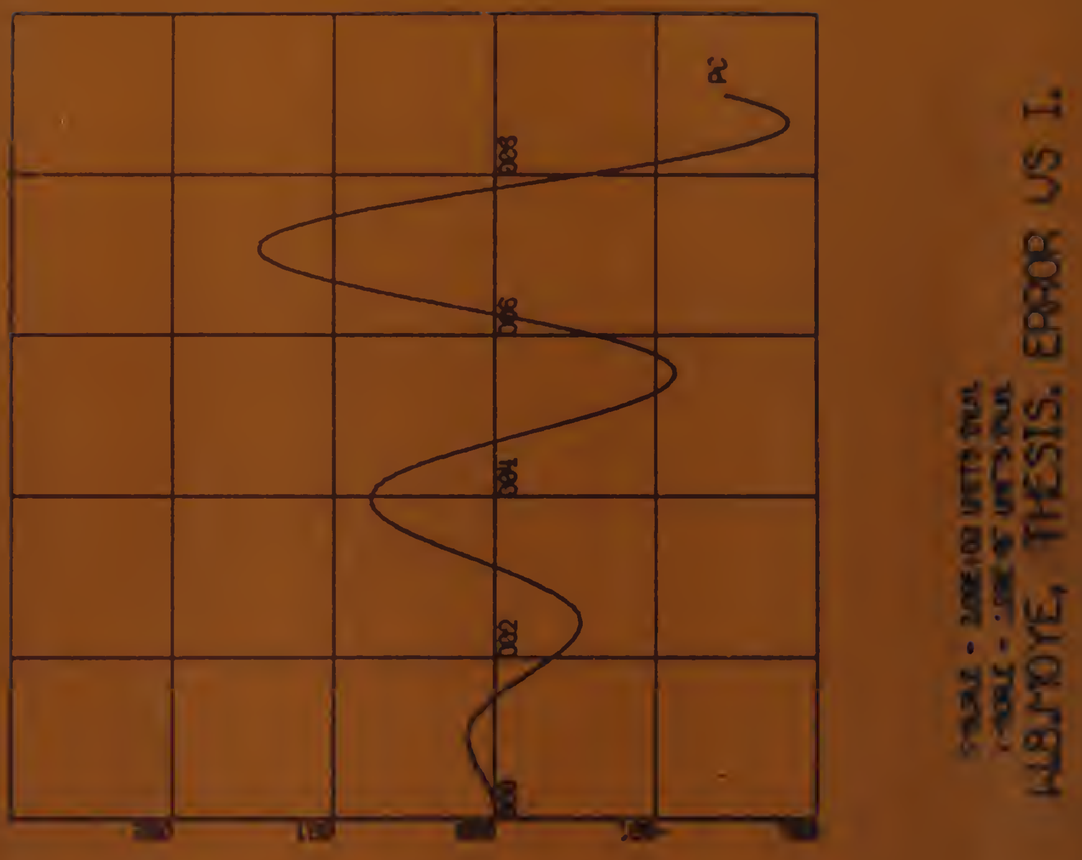
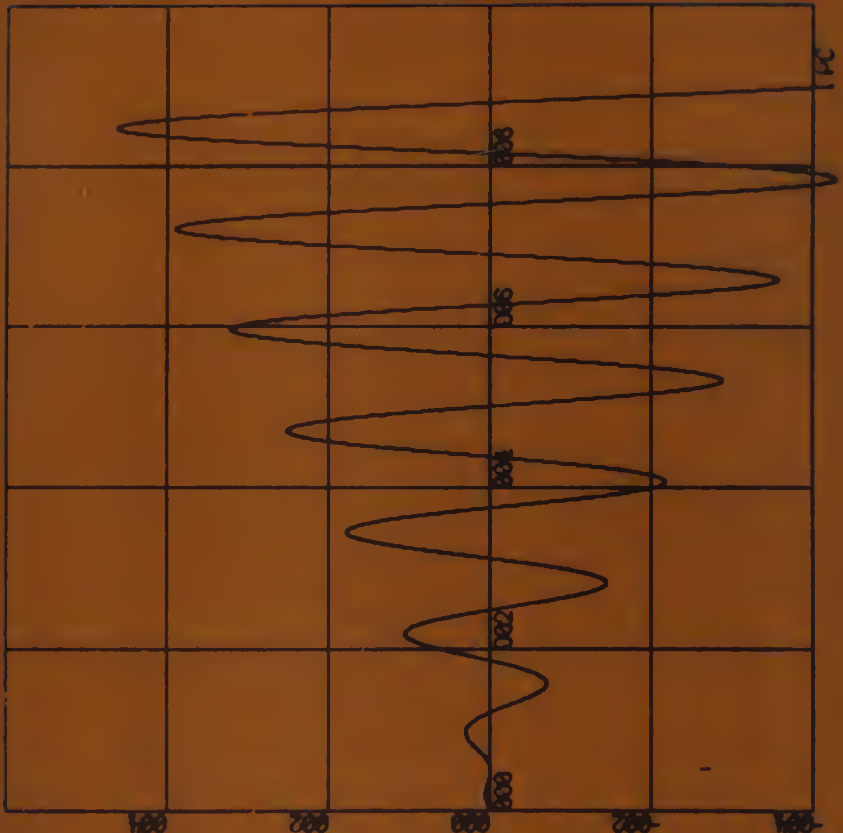


Fig. [illegible] Error
Step length = .03



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Rational Pade' convergents to a function of the forward shift operator E are computed from coefficients of its power series expansion. These Pade' convergents are used to generate recursion formulas which are then employed to obtain approximate numerical solutions of several second order differential equations. A variety of integration step lengths are used. Solution error is plotted against the number of iteration steps and results are evaluated. It is concluded that this procedure is beneficial as a method of deriving corrector formulas to be used in the predictor-corrector method of solving second order differential equations. A method for deriving improved predictor formulas is suggested.

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